



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:04 PM GMT

PDB ID : 4YBB
Title : High-resolution structure of the Escherichia coli ribosome
Authors : Noeske, J.; Wasserman, M.R.; Terry, D.S.; Altman, R.B.; Blanchard, S.C.;
Cate, J.H.D.
Deposited on : 2015-02-18
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

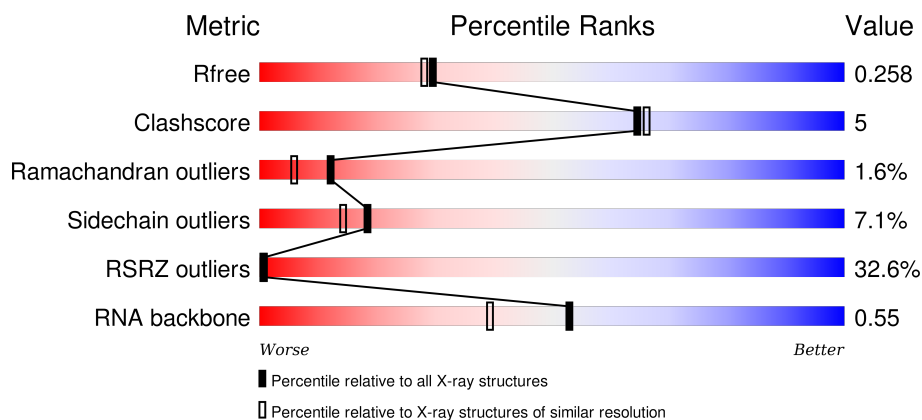
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 3939 (2.10-2.10) |
| Clashscore | 102246 | 4460 (2.10-2.10) |
| Ramachandran outliers | 100387 | 4413 (2.10-2.10) |
| Sidechain outliers | 100360 | 4414 (2.10-2.10) |
| RSRZ outliers | 91569 | 3948 (2.10-2.10) |
| RNA backbone | 2183 | 1118 (2.80-1.40) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | AA | 1534 | <div> <div>7%</div> <div>73%</div> <div>21%</div> <div>5%</div> </div> |
| 1 | BA | 1534 | <div> <div>21%</div> <div>69%</div> <div>24%</div> <div>5%</div> </div> |
| 2 | AB | 224 | <div> <div>63%</div> <div>82%</div> <div>16%</div> </div> |
| 2 | BB | 224 | <div> <div>73%</div> <div>79%</div> <div>19%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | AC | 206 | |
| 3 | BC | 206 | |
| 4 | AD | 205 | |
| 4 | BD | 205 | |
| 5 | AE | 155 | |
| 5 | BE | 155 | |
| 6 | AF | 106 | |
| 6 | BF | 106 | |
| 7 | AG | 151 | |
| 7 | BG | 151 | |
| 8 | AH | 129 | |
| 8 | BH | 129 | |
| 9 | AI | 127 | |
| 9 | BI | 127 | |
| 10 | AJ | 99 | |
| 10 | BJ | 99 | |
| 11 | AK | 117 | |
| 11 | BK | 117 | |
| 12 | AL | 123 | |
| 12 | BL | 123 | |
| 13 | AM | 114 | |
| 13 | BM | 114 | |
| 14 | AN | 100 | |
| 14 | BN | 100 | |
| 15 | AO | 88 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15 | BO | 88 | |
| 16 | AP | 82 | |
| 16 | BP | 82 | |
| 17 | AQ | 80 | |
| 17 | BQ | 80 | |
| 18 | AR | 55 | |
| 18 | BR | 55 | |
| 19 | AS | 79 | |
| 19 | BS | 79 | |
| 20 | AT | 86 | |
| 20 | BT | 86 | |
| 21 | AU | 56 | |
| 21 | BU | 56 | |
| 22 | CA | 2904 | |
| 23 | CB | 120 | |
| 23 | DB | 120 | |
| 24 | CC | 271 | |
| 24 | DC | 271 | |
| 25 | CD | 209 | |
| 26 | CE | 201 | |
| 26 | DE | 201 | |
| 27 | CF | 177 | |
| 27 | DF | 177 | |
| 28 | CG | 176 | |
| 28 | DG | 176 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------------|
| 29 | CH | 149 | <div>79%</div> <div>72% 23% 5%</div> |
| 29 | DH | 149 | <div>70%</div> <div>81% 17%</div> |
| 30 | CJ | 134 | <div>100%</div> <div>75% 24%</div> |
| 30 | DJ | 134 | <div>98%</div> <div>77% 22%</div> |
| 31 | CK | 142 | <div>58%</div> <div>78% 18%</div> |
| 31 | DK | 142 | <div>18%</div> <div>93% 7%</div> |
| 32 | CL | 123 | <div>44%</div> <div>72% 24%</div> |
| 32 | DL | 123 | <div>7%</div> <div>87% 11%</div> |
| 33 | CM | 144 | <div>83%</div> <div>75% 20%</div> |
| 33 | DM | 144 | <div>22%</div> <div>87% 13%</div> |
| 34 | CN | 136 | <div>43%</div> <div>88% 10%</div> |
| 34 | DN | 136 | <div>4%</div> <div>90% 10%</div> |
| 35 | CO | 125 | <div>63%</div> <div>71% 18% 6%</div> |
| 35 | DO | 125 | <div>22%</div> <div>90% 9%</div> |
| 36 | CP | 117 | <div>91%</div> <div>74% 22%</div> |
| 36 | DP | 117 | <div>2%</div> <div>91% 8%</div> |
| 37 | CQ | 114 | <div>62%</div> <div>83% 15%</div> |
| 37 | DQ | 114 | <div>12%</div> <div>89% 10%</div> |
| 38 | CR | 117 | <div>61%</div> <div>78% 20%</div> |
| 38 | DR | 117 | <div>31%</div> <div>91% 9%</div> |
| 39 | CS | 103 | <div>71%</div> <div>79% 18%</div> |
| 39 | DS | 103 | <div>11%</div> <div>88% 12%</div> |
| 40 | CT | 110 | <div>71%</div> <div>83% 13% 5%</div> |
| 40 | DT | 110 | <div>11%</div> <div>95% 5%</div> |
| 41 | CU | 93 | <div>88%</div> <div>77% 13% 9%</div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 41 | DU | 93 | |
| 42 | CV | 102 | |
| 42 | DV | 102 | |
| 43 | CW | 94 | |
| 43 | DW | 94 | |
| 44 | CX | 76 | |
| 44 | DX | 76 | |
| 45 | CY | 77 | |
| 45 | DY | 77 | |
| 46 | CZ | 62 | |
| 46 | DZ | 62 | |
| 47 | C0 | 58 | |
| 47 | D0 | 58 | |
| 48 | C1 | 56 | |
| 48 | D1 | 56 | |
| 49 | C2 | 51 | |
| 49 | D2 | 51 | |
| 50 | C3 | 46 | |
| 50 | D3 | 46 | |
| 51 | C4 | 64 | |
| 51 | D4 | 64 | |
| 52 | C5 | 38 | |
| 52 | D5 | 38 | |
| 53 | DA | 2903 | |
| 54 | DD | 209 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 55 | DI | 135 | <div> <div>88%</div> <div>72%26%..</div> </div> |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | AA | 1603 | - | - | - | X |
| 56 | MG | AA | 1608 | - | - | - | X |
| 56 | MG | AA | 1611 | - | - | - | X |
| 56 | MG | AA | 1612 | - | - | - | X |
| 56 | MG | AA | 1631 | - | - | - | X |
| 56 | MG | AA | 1642 | - | - | - | X |
| 56 | MG | AA | 1661 | - | - | - | X |
| 56 | MG | BA | 1605 | - | - | - | X |
| 56 | MG | BA | 1624 | - | - | - | X |
| 56 | MG | BA | 1632 | - | - | - | X |
| 56 | MG | CA | 3002 | - | - | - | X |
| 56 | MG | CA | 3005 | - | - | - | X |
| 56 | MG | CA | 3025 | - | - | - | X |
| 56 | MG | CA | 3036 | - | - | - | X |
| 56 | MG | CA | 3132 | - | - | - | X |
| 56 | MG | CA | 3150 | - | - | - | X |
| 56 | MG | CB | 202 | - | - | - | X |
| 56 | MG | DA | 3006 | - | - | - | X |
| 56 | MG | DA | 3011 | - | - | - | X |
| 56 | MG | DA | 3015 | - | - | - | X |
| 56 | MG | DA | 3022 | - | - | - | X |
| 56 | MG | DA | 3027 | - | - | - | X |
| 56 | MG | DA | 3033 | - | - | - | X |
| 56 | MG | DA | 3035 | - | - | - | X |
| 56 | MG | DA | 3044 | - | - | - | X |
| 56 | MG | DA | 3045 | - | - | - | X |
| 56 | MG | DA | 3048 | - | - | - | X |
| 56 | MG | DA | 3057 | - | - | - | X |
| 56 | MG | DA | 3064 | - | - | - | X |
| 56 | MG | DA | 3069 | - | - | - | X |
| 56 | MG | DA | 3088 | - | - | - | X |
| 56 | MG | DA | 3090 | - | - | - | X |
| 56 | MG | DA | 3091 | - | - | - | X |
| 56 | MG | DA | 3108 | - | - | - | X |
| 56 | MG | DA | 3119 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 56 | MG | DA | 3122 | - | - | - | X |
| 56 | MG | DA | 3125 | - | - | - | X |
| 56 | MG | DA | 3126 | - | - | - | X |
| 56 | MG | DA | 3172 | - | - | - | X |
| 56 | MG | DA | 3177 | - | - | - | X |
| 57 | PG4 | DA | 3193 | - | - | X | X |
| 57 | PG4 | DR | 202 | - | - | X | X |
| 58 | MPD | AA | 1671 | - | - | - | X |
| 58 | MPD | AA | 1676 | - | - | - | X |
| 58 | MPD | DA | 3192 | - | - | - | X |
| 58 | MPD | DA | 3205 | - | - | - | X |
| 58 | MPD | DA | 3208 | - | - | - | X |
| 58 | MPD | DE | 301 | - | - | - | X |
| 58 | MPD | DN | 201 | - | - | X | - |
| 59 | PUT | AA | 1672 | - | - | - | X |
| 59 | PUT | DA | 3184 | - | - | - | X |
| 59 | PUT | DA | 3189 | - | - | - | X |
| 59 | PUT | DA | 3214 | - | - | - | X |
| 59 | PUT | DA | 3220 | - | - | - | X |
| 59 | PUT | DA | 3222 | - | - | - | X |
| 59 | PUT | DA | 3223 | - | - | X | X |
| 59 | PUT | DM | 201 | - | - | - | X |
| 60 | ZN | AB | 301 | - | - | - | X |
| 61 | PEG | D3 | 102 | - | - | X | X |
| 61 | PEG | DA | 3200 | - | - | - | X |
| 61 | PEG | DA | 3219 | - | - | - | X |
| 61 | PEG | DP | 201 | - | - | X | - |
| 62 | SPD | DA | 3187 | - | - | - | X |
| 62 | SPD | DA | 3225 | - | - | - | X |
| 64 | PGE | D1 | 102 | - | - | - | X |
| 64 | PGE | DA | 3186 | - | - | - | X |
| 65 | ACY | DA | 3202 | - | - | - | X |
| 66 | EDO | D0 | 101 | - | - | - | X |
| 66 | EDO | DA | 3198 | - | - | - | X |

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295060 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1 | AA | 1534 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32930 | 14694 | 6041 | 10661 | 1534 | | | |
| 1 | BA | 1533 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 32908 | 14684 | 6036 | 10655 | 1533 | | | |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | AB | 224 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1753 | 1109 | 315 | 321 | 8 | | | |
| 2 | BB | 224 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1753 | 1109 | 315 | 321 | 8 | | | |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | AC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1625 | 1028 | 305 | 289 | 3 | | | |
| 3 | BC | 206 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1625 | 1028 | 305 | 289 | 3 | | | |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | AD | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | | |
| 4 | BD | 205 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1643 | 1026 | 315 | 298 | 4 | | | |

- Molecule 5 is a protein called 30S ribosomal protein S5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5 | AE | 155 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1144 | 711 | 216 | 211 | 6 | | | |
| 5 | BE | 150 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1105 | 687 | 211 | 201 | 6 | | | |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6 | AF | 106 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 862 | 545 | 156 | 154 | 7 | | | |
| 6 | BF | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 817 | 515 | 148 | 148 | 6 | | | |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7 | AG | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1182 | 735 | 227 | 216 | 4 | | | |
| 7 | BG | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1182 | 735 | 227 | 216 | 4 | | | |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8 | AH | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | | |
| 8 | BH | 129 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 616 | 173 | 184 | 6 | | | |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9 | AI | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | | |
| 9 | BI | 127 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1022 | 634 | 206 | 179 | 3 | | | |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | AJ | 99 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 796 | 498 | 152 | 145 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10 | BJ | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 787 | 493 | 150 | 143 | 1 | | | |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11 | AK | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |
| 11 | BK | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 877 | 540 | 174 | 160 | 3 | | | |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12 | AL | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 957 | 591 | 196 | 165 | 5 | | | |
| 12 | BL | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 957 | 591 | 196 | 165 | 5 | | | |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13 | AM | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 884 | 546 | 178 | 157 | 3 | | | |
| 13 | BM | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 884 | 546 | 178 | 157 | 3 | | | |

- Molecule 14 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | AN | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 805 | 499 | 164 | 139 | 3 | | | |
| 14 | BN | 100 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 805 | 499 | 164 | 139 | 3 | | | |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15 | AO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | | |
| 15 | BO | 88 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 714 | 439 | 144 | 130 | 1 | | | |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | AP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | | |
| 16 | BP | 82 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 406 | 128 | 114 | 1 | | | |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17 | AQ | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 411 | 121 | 114 | 3 | | | |
| 17 | BQ | 80 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 649 | 411 | 121 | 114 | 3 | | | |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 18 | AR | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 456 | 288 | 86 | 82 | | | |
| 18 | BR | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 456 | 288 | 86 | 82 | | | |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19 | AS | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 638 | 408 | 120 | 108 | 2 | | | |
| 19 | BS | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 638 | 408 | 120 | 108 | 2 | | | |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20 | AT | 86 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 670 | 414 | 138 | 115 | 3 | | | |
| 20 | BT | 85 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 665 | 411 | 137 | 114 | 3 | | | |

- Molecule 21 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 21 | AU | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 465 | 290 | 96 | 78 | 1 | | | |
| 21 | BU | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 465 | 290 | 96 | 78 | 1 | | | |

- Molecule 22 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 22 | CA | 2898 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 62229 | 27768 | 11448 | 20115 | 2898 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|--------------|
| CA | 2798 | U | UNK | conflict | GB 731469900 |
| CA | 2800 | A | UNK | conflict | GB 731469900 |

- Molecule 23 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 23 | CB | 118 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2529 | 1126 | 464 | 821 | 118 | | | |
| 23 | DB | 120 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 2569 | 1144 | 468 | 837 | 120 | | | |

- Molecule 24 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 24 | CC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2083 | 1288 | 423 | 365 | 7 | | | |
| 24 | DC | 271 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2083 | 1288 | 423 | 365 | 7 | | | |

- Molecule 25 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25 | CD | 209 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1565 | 979 | 288 | 294 | 4 | | | |

- Molecule 26 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26 | CE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |
| 26 | DE | 201 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1552 | 974 | 283 | 290 | 5 | | | |

- Molecule 27 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27 | CF | 177 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1411 | 899 | 249 | 257 | 6 | | | |
| 27 | DF | 177 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1411 | 899 | 249 | 257 | 6 | | | |

- Molecule 28 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28 | CG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |
| 28 | DG | 176 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1323 | 832 | 243 | 246 | 2 | | | |

- Molecule 29 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29 | CH | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 699 | 197 | 213 | 1 | | | |
| 29 | DH | 149 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 699 | 197 | 213 | 1 | | | |

- Molecule 30 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30 | CJ | 134 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 619 | 169 | 185 | 6 | | | |
| 30 | DJ | 134 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 979 | 619 | 169 | 185 | 6 | | | |

- Molecule 31 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | CK | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31 | DK | 142 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1129 | 714 | 212 | 199 | 4 | | | |

- Molecule 32 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32 | CL | 122 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 938 | 587 | 180 | 165 | 6 | | | |
| 32 | DL | 123 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 946 | 593 | 181 | 166 | 6 | | | |

- Molecule 33 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33 | CM | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1053 | 654 | 207 | 190 | 2 | | | |
| 33 | DM | 144 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1053 | 654 | 207 | 190 | 2 | | | |

- Molecule 34 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34 | CN | 136 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1075 | 686 | 205 | 178 | 6 | | | |
| 34 | DN | 136 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 1092 | 696 | 211 | 179 | 6 | | | |

- Molecule 35 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35 | CO | 120 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 960 | 593 | 196 | 166 | 5 | | | |
| 35 | DO | 125 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 993 | 613 | 202 | 173 | 5 | | | |

- Molecule 36 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 36 | CP | 116 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 892 | 552 | 178 | 162 | | | | |
| 36 | DP | 117 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 900 | 557 | 179 | 163 | 1 | | | |

- Molecule 37 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37 | CQ | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | | |
| 37 | DQ | 114 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 917 | 574 | 179 | 163 | 1 | | | |

- Molecule 38 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 38 | CR | 117 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | | |
| 38 | DR | 117 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 947 | 604 | 192 | 151 | | | | |

- Molecule 39 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39 | CS | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | | |
| 39 | DS | 103 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 816 | 516 | 153 | 145 | 2 | | | |

- Molecule 40 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40 | CT | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | | |
| 40 | DT | 110 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 857 | 532 | 166 | 156 | 3 | | | |

- Molecule 41 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41 | CU | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 739 | 466 | 139 | 132 | 2 | | | |
| 41 | DU | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 739 | 466 | 139 | 132 | 2 | | | |

- Molecule 42 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 42 | CV | 102 | Total | C | N | O | 0 | 0 | 0 |
| | | | 780 | 492 | 146 | 142 | | | |
| 42 | DV | 102 | Total | C | N | O | 0 | 0 | 0 |
| | | | 780 | 492 | 146 | 142 | | | |

- Molecule 43 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 43 | CW | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |
| 43 | DW | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 753 | 479 | 137 | 134 | 3 | | | |

- Molecule 44 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 44 | CX | 75 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 569 | 353 | 113 | 102 | 1 | | | |
| 44 | DX | 76 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 591 | 365 | 121 | 104 | 1 | | | |

- Molecule 45 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 45 | CY | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |
| 45 | DY | 77 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 625 | 388 | 129 | 106 | 2 | | | |

- Molecule 46 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 46 | CZ | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 501 | 308 | 98 | 94 | 1 | | | |
| 46 | DZ | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 501 | 308 | 98 | 94 | 1 | | | |

- Molecule 47 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 47 | C0 | 58 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 449 | 281 | 87 | 79 | 2 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 47 | D0 | 58 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 463 | 290 | 90 | 81 | 2 | | | |

- Molecule 48 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 48 | C1 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |
| 48 | D1 | 56 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 444 | 269 | 94 | 80 | 1 | | | |

- Molecule 49 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 49 | C2 | 50 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 409 | 263 | 75 | 71 | | | | |
| 49 | D2 | 51 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 414 | 266 | 76 | 72 | | | | |

- Molecule 50 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50 | C3 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |
| 50 | D3 | 46 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 377 | 228 | 90 | 57 | 2 | | | |

- Molecule 51 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 51 | C4 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |
| 51 | D4 | 64 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 504 | 323 | 105 | 74 | 2 | | | |

- Molecule 52 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52 | C5 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |
| 52 | D5 | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 302 | 185 | 65 | 48 | 4 | | | |

- Molecule 53 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 53 | DA | 2897 | Total | C | N | O | P | 0 | 8 | 0 |
| | | | 62361 | 27827 | 11476 | 20154 | 2904 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|--------------|
| DA | 2798 | U | UNK | conflict | GB 731469900 |
| DA | 2800 | A | UNK | conflict | GB 731469900 |

- Molecule 54 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 54 | DD | 209 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 1576 | 986 | 290 | 296 | 4 | | | |

- Molecule 55 is a protein called 50S ribosomal protein L10.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 55 | DI | 135 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1023 | 649 | 179 | 192 | 3 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| DI | 85 | VAL | SER | conflict | UNP P0A7J3 |
| DI | 86 | THR | MET | conflict | UNP P0A7J3 |

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

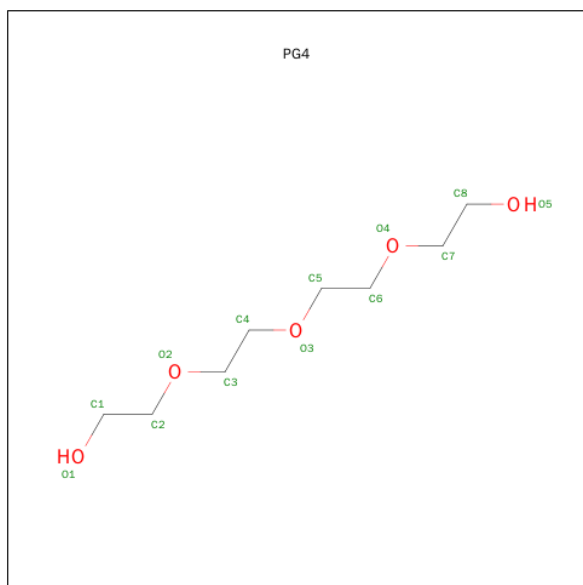
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 56 | BA | 41 | Total | Mg | 0 | 0 |
| | | | 41 | 41 | | |
| 56 | CA | 155 | Total | Mg | 0 | 0 |
| | | | 155 | 155 | | |
| 56 | CB | 3 | Total | Mg | 0 | 0 |
| | | | 3 | 3 | | |
| 56 | DR | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | AA | 70 | Total | Mg | 0 | 0 |
| | | | 70 | 70 | | |

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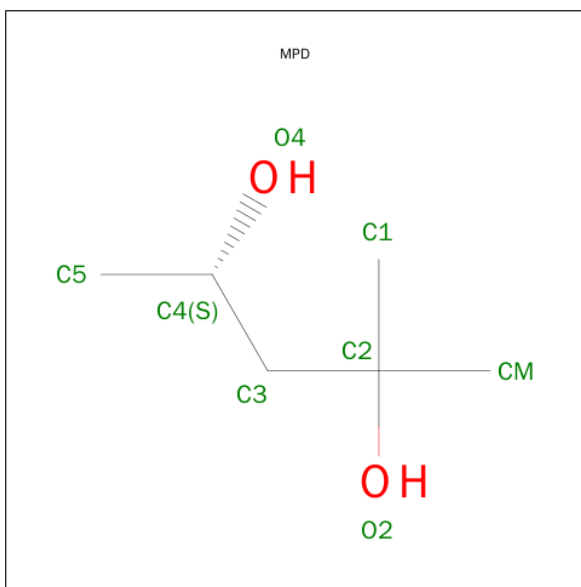
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 56 | DA | 183 | Total | Mg | 0 | 0 |
| | | | 183 | 183 | | |
| 56 | C3 | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 56 | DB | 9 | Total | Mg | 0 | 0 |
| | | | 9 | 9 | | |

- Molecule 57 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



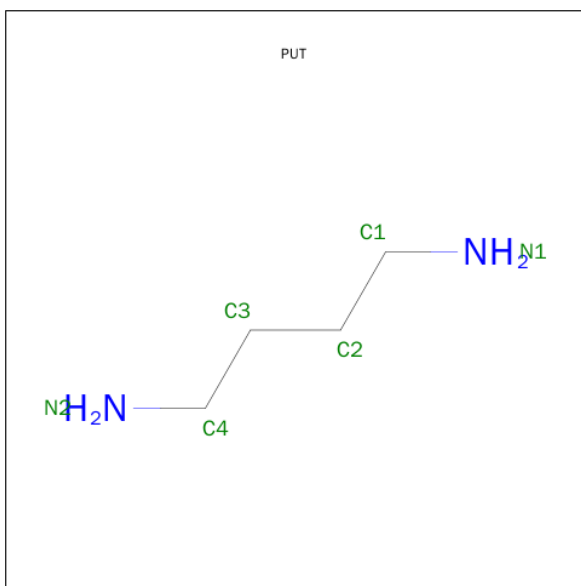
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 57 | AA | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 8 | 5 | | |
| 57 | BA | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 8 | 5 | | |
| 57 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 8 | 5 | | |
| 57 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 8 | 5 | | |
| 57 | DQ | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 8 | 5 | | |
| 57 | DR | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 8 | 5 | | |
| 57 | DS | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 8 | 5 | | |

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 58 | AA | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | AA | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DE | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DE | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DK | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DN | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DS | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DT | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 58 | DT | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |

- Molecule 59 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula: C₄H₁₂N₂).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 59 | AA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | AA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | AA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | AA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |

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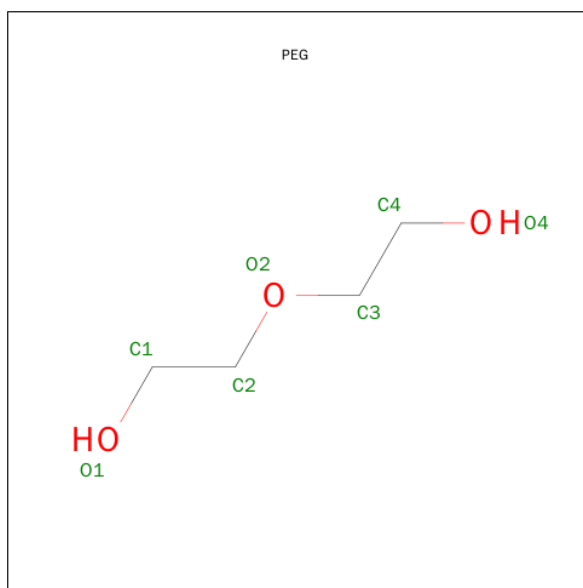
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 59 | DM | 1 | Total | C | N | 0 | 0 |
| | | | 6 | 4 | 2 | | |

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 60 | C5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | AB | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |
| 60 | D5 | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 61 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



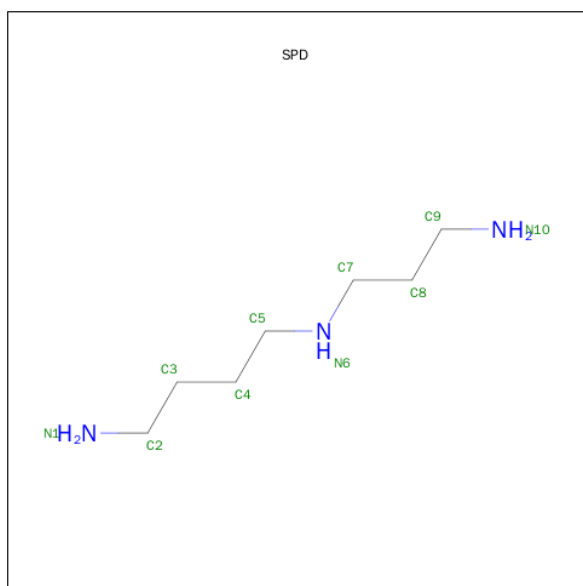
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 61 | AL | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 61 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 61 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 61 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 61 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 61 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 61 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 61 | DL | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 61 | DP | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 61 | DQ | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 61 | D3 | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |

- Molecule 62 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



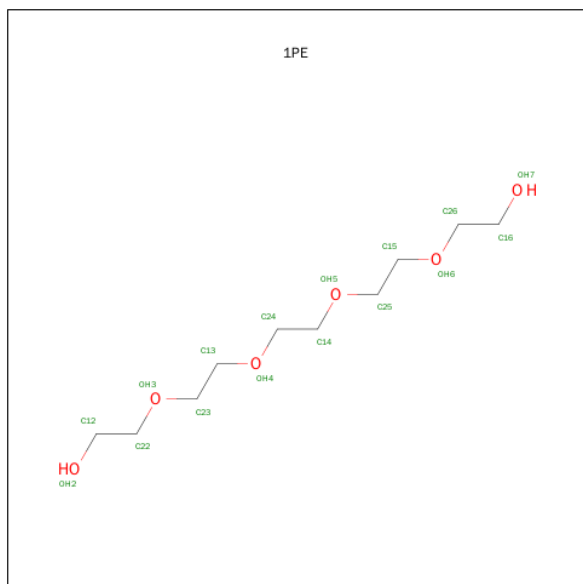
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 62 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 62 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 62 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 10 | 7 | 3 | | |

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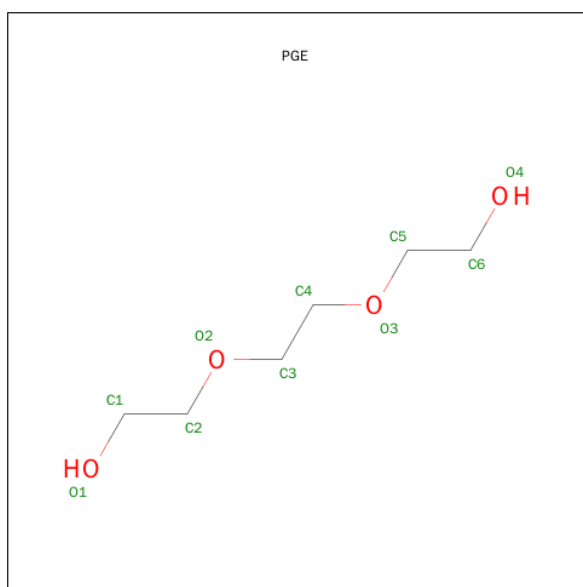
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 62 | DA | 1 | Total | C | N | 0 | 0 |
| | | | 10 | 7 | 3 | | |

- Molecule 63 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



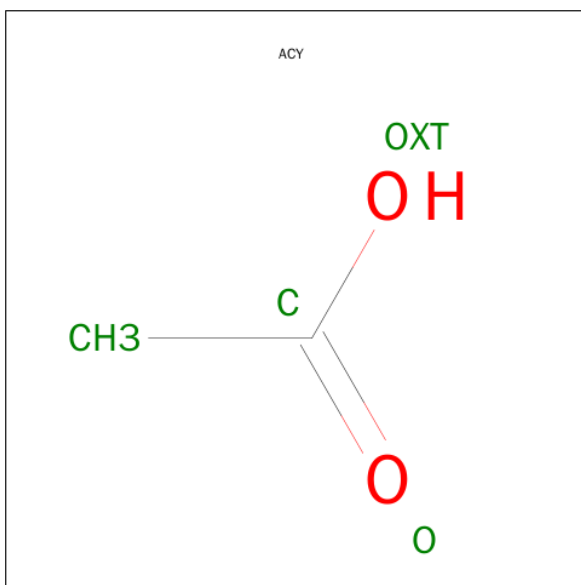
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 63 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 16 | 10 | 6 | | |
| 63 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 16 | 10 | 6 | | |

- Molecule 64 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



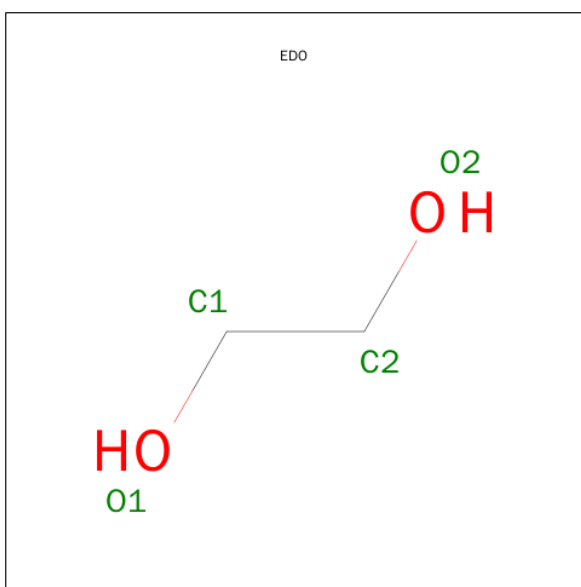
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 64 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 64 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 64 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 64 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 64 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 64 | DS | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 64 | DU | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 64 | D1 | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 64 | D3 | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |

- Molecule 65 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 65 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 65 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 65 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |

- Molecule 66 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



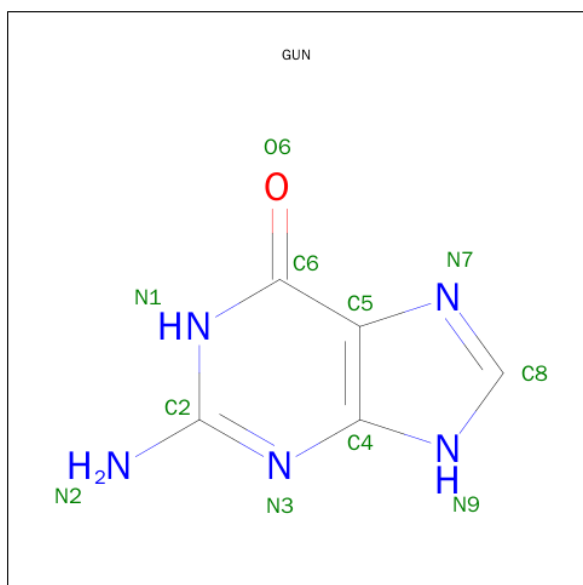
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 66 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |

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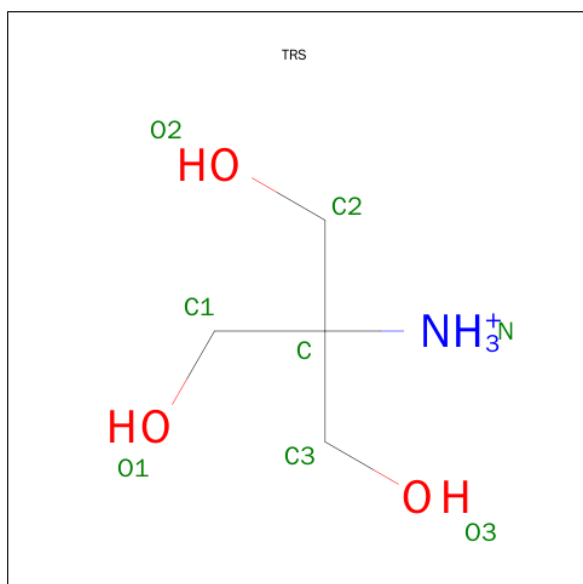
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 66 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 66 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 66 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 66 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 66 | DA | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 66 | DB | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 66 | DB | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 66 | DB | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 66 | DR | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 66 | D0 | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 66 | D1 | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |

- Molecule 67 is GUANINE (three-letter code: GUN) (formula: $C_5H_5N_5O$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 67 | DA | 1 | Total | C | N | O | 0 | 0 |
| | | | 11 | 5 | 5 | 1 | | |

- Molecule 68 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 68 | DA | 1 | Total | C | N | O | 0 | 0 |
| | | | 8 | 4 | 1 | 3 | | |

- Molecule 69 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 69 | AA | 509 | Total | O | 0 | 0 |
| | | | 509 | 509 | | |
| 69 | AC | 6 | Total | O | 0 | 0 |
| | | | 6 | 6 | | |
| 69 | AD | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 69 | AE | 5 | Total | O | 0 | 0 |
| | | | 5 | 5 | | |
| 69 | AF | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 69 | AG | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 69 | AH | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 69 | AJ | 2 | Total 2 | O 2 | 0 | 0 |
| 69 | AK | 6 | Total 6 | O 6 | 0 | 0 |
| 69 | AL | 10 | Total 10 | O 10 | 0 | 0 |
| 69 | AM | 4 | Total 4 | O 4 | 0 | 0 |
| 69 | AN | 6 | Total 6 | O 6 | 0 | 0 |
| 69 | AO | 2 | Total 2 | O 2 | 0 | 0 |
| 69 | AP | 2 | Total 2 | O 2 | 0 | 0 |
| 69 | AS | 1 | Total 1 | O 1 | 0 | 0 |
| 69 | AT | 2 | Total 2 | O 2 | 0 | 0 |
| 69 | AU | 2 | Total 2 | O 2 | 0 | 0 |
| 69 | BA | 286 | Total 286 | O 286 | 0 | 0 |
| 69 | BD | 12 | Total 12 | O 12 | 0 | 0 |
| 69 | BE | 1 | Total 1 | O 1 | 0 | 0 |
| 69 | BF | 2 | Total 2 | O 2 | 0 | 0 |
| 69 | BL | 5 | Total 5 | O 5 | 0 | 0 |
| 69 | BN | 3 | Total 3 | O 3 | 0 | 0 |
| 69 | BO | 1 | Total 1 | O 1 | 0 | 0 |
| 69 | BP | 3 | Total 3 | O 3 | 0 | 0 |
| 69 | BT | 5 | Total 5 | O 5 | 0 | 0 |
| 69 | BU | 2 | Total 2 | O 2 | 0 | 0 |
| 69 | CA | 692 | Total 692 | O 692 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 69 | CB | 13 | Total 13 | O 13 | 0 | 0 |
| 69 | CC | 8 | Total 8 | O 8 | 0 | 0 |
| 69 | CD | 6 | Total 6 | O 6 | 0 | 0 |
| 69 | CE | 6 | Total 6 | O 6 | 0 | 0 |
| 69 | CK | 1 | Total 1 | O 1 | 0 | 0 |
| 69 | CL | 1 | Total 1 | O 1 | 0 | 0 |
| 69 | CM | 5 | Total 5 | O 5 | 0 | 0 |
| 69 | CO | 1 | Total 1 | O 1 | 0 | 0 |
| 69 | CS | 1 | Total 1 | O 1 | 0 | 0 |
| 69 | CU | 2 | Total 2 | O 2 | 0 | 0 |
| 69 | CV | 2 | Total 2 | O 2 | 0 | 0 |
| 69 | CW | 1 | Total 1 | O 1 | 0 | 0 |
| 69 | CY | 1 | Total 1 | O 1 | 0 | 0 |
| 69 | C3 | 2 | Total 2 | O 2 | 0 | 0 |
| 69 | C4 | 1 | Total 1 | O 1 | 0 | 0 |
| 69 | DA | 4815 | Total 4815 | O 4815 | 0 | 0 |
| 69 | DB | 209 | Total 209 | O 209 | 0 | 0 |
| 69 | DC | 106 | Total 106 | O 106 | 0 | 0 |
| 69 | DD | 103 | Total 103 | O 103 | 0 | 0 |
| 69 | DE | 62 | Total 62 | O 62 | 0 | 0 |
| 69 | DF | 14 | Total 14 | O 14 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 69 | DG | 6 | Total 6 | O 6 | 0 | 0 |
| 69 | DH | 2 | Total 2 | O 2 | 0 | 0 |
| 69 | DK | 59 | Total 59 | O 59 | 0 | 0 |
| 69 | DL | 45 | Total 45 | O 45 | 0 | 0 |
| 69 | DM | 67 | Total 67 | O 67 | 0 | 0 |
| 69 | DN | 74 | Total 74 | O 74 | 0 | 0 |
| 69 | DO | 42 | Total 42 | O 42 | 0 | 0 |
| 69 | DP | 37 | Total 37 | O 37 | 0 | 0 |
| 69 | DQ | 27 | Total 27 | O 27 | 0 | 0 |
| 69 | DR | 67 | Total 67 | O 67 | 0 | 0 |
| 69 | DS | 50 | Total 50 | O 50 | 0 | 0 |
| 69 | DT | 61 | Total 61 | O 61 | 0 | 0 |
| 69 | DU | 19 | Total 19 | O 19 | 0 | 0 |
| 69 | DV | 22 | Total 22 | O 22 | 0 | 0 |
| 69 | DW | 32 | Total 32 | O 32 | 0 | 0 |
| 69 | DX | 30 | Total 30 | O 30 | 0 | 0 |
| 69 | DY | 10 | Total 10 | O 10 | 0 | 0 |
| 69 | DZ | 8 | Total 8 | O 8 | 0 | 0 |
| 69 | D0 | 25 | Total 25 | O 25 | 0 | 0 |
| 69 | D1 | 47 | Total 47 | O 47 | 0 | 0 |
| 69 | D2 | 9 | Total 9 | O 9 | 0 | 0 |

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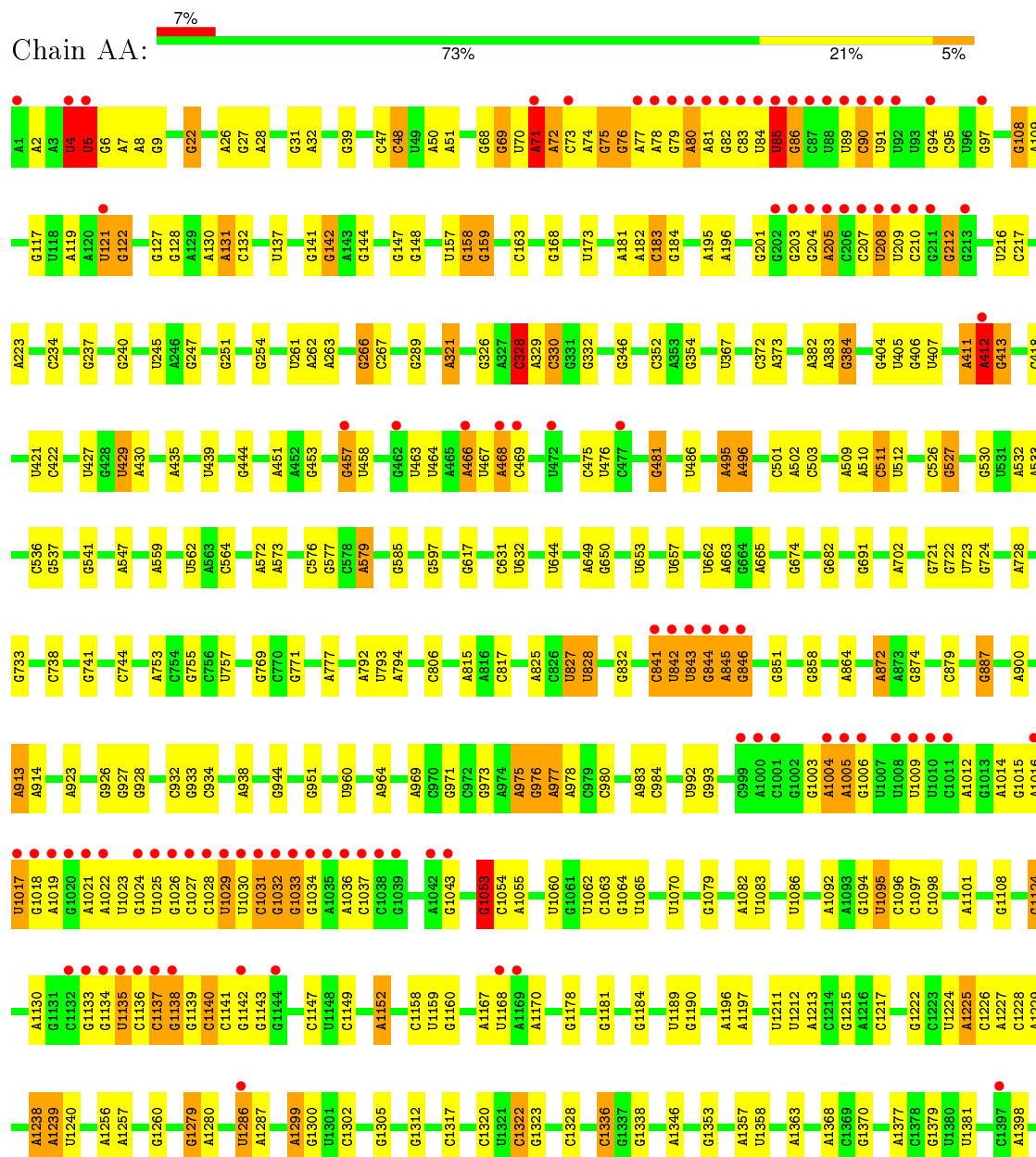
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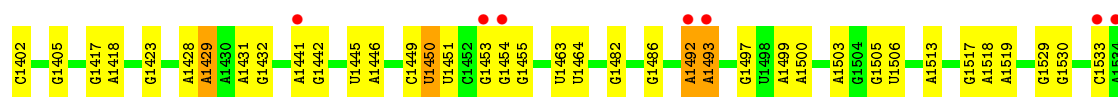
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 69 | D3 | 25 | Total 25 | O 25 | 0 | 0 |
| 69 | D4 | 38 | Total 38 | O 38 | 0 | 0 |
| 69 | D5 | 14 | Total 14 | O 14 | 0 | 0 |

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

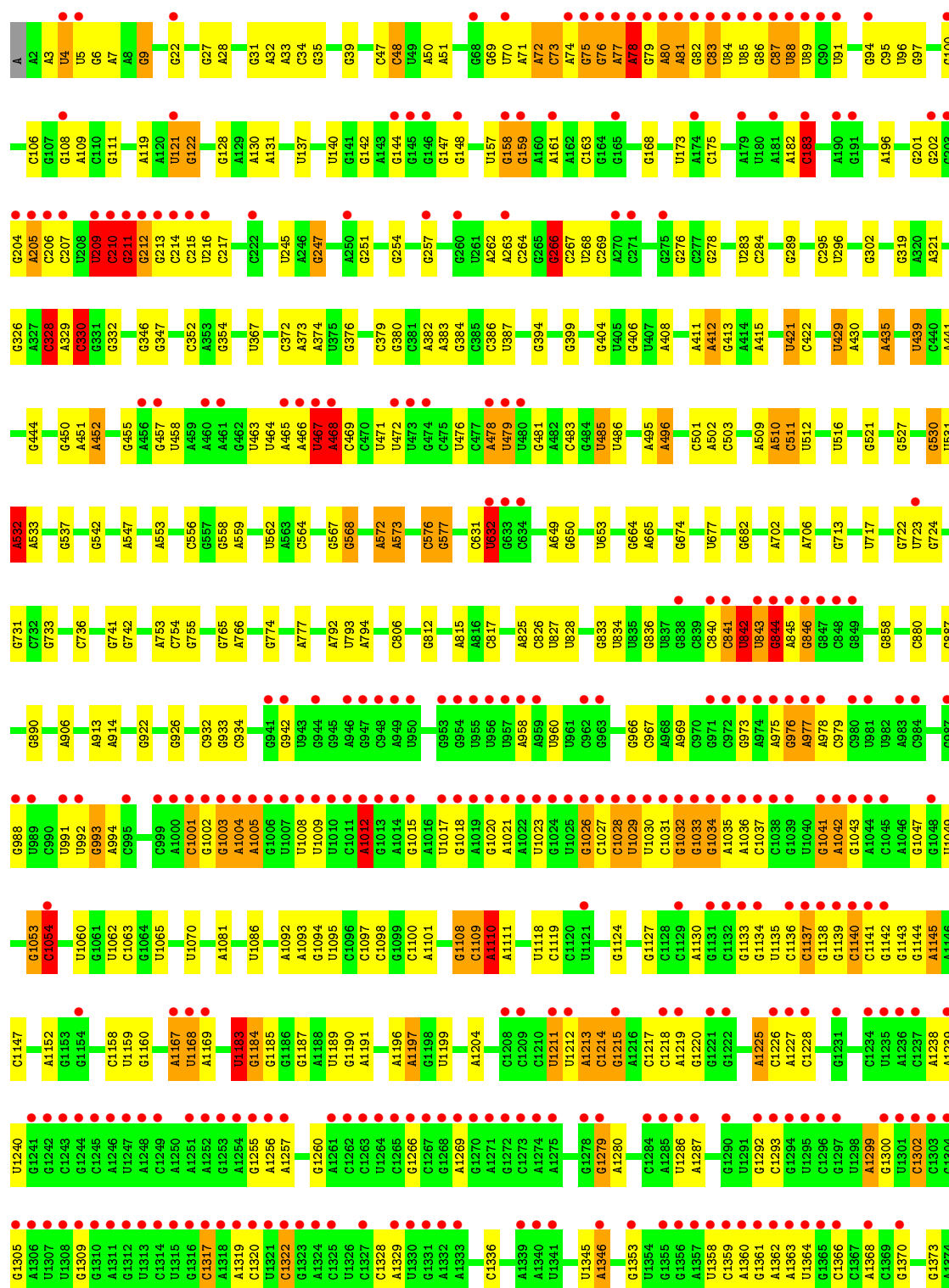
• Molecule 1: 16S rRNA

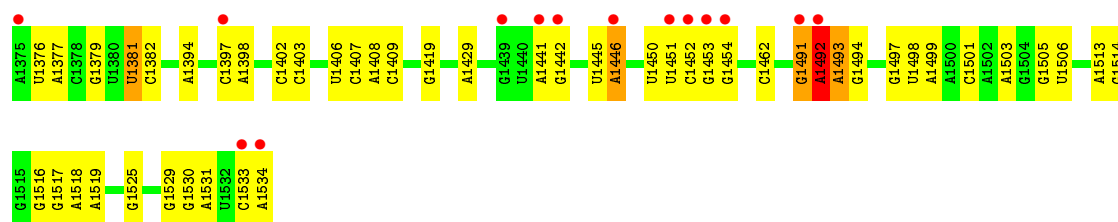




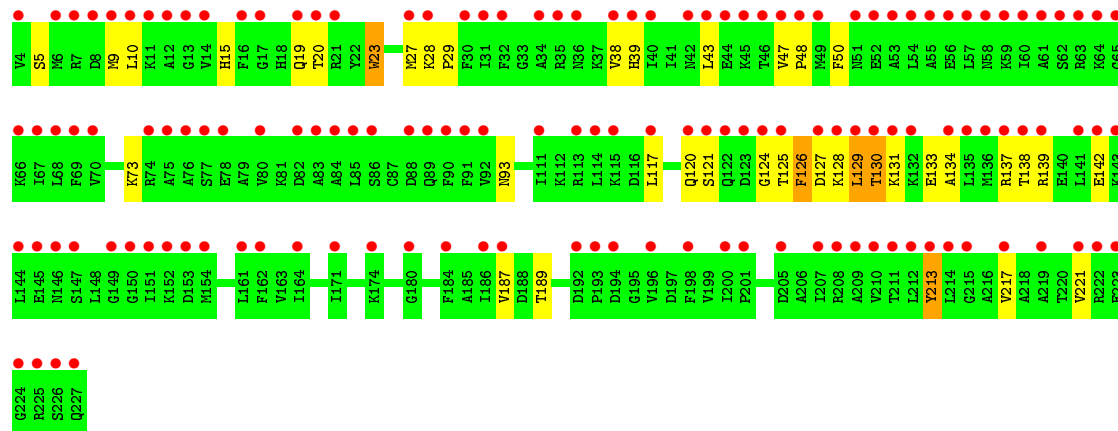
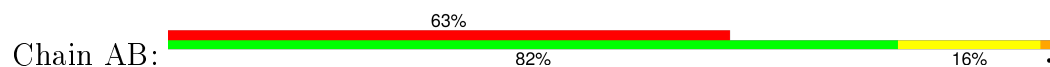
• Molecule 1: 16S rRNA

Chain BA: 21% 69% 24% 5%

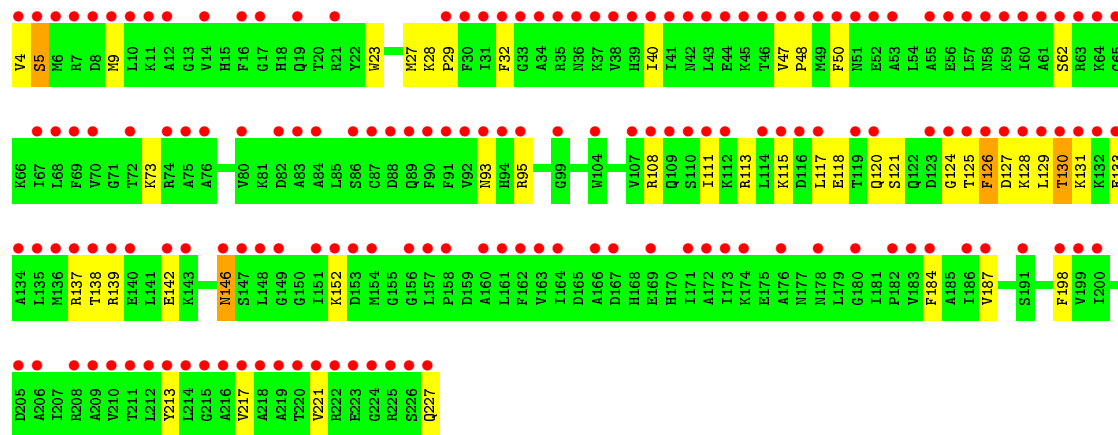
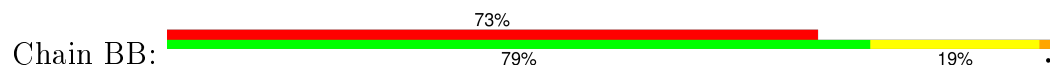




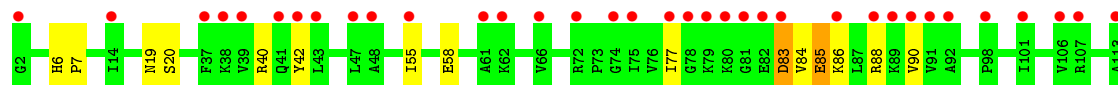
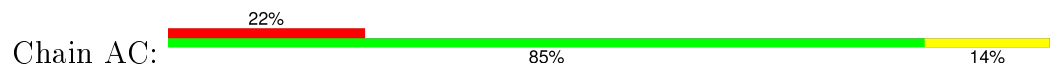
• Molecule 2: 30S ribosomal protein S2

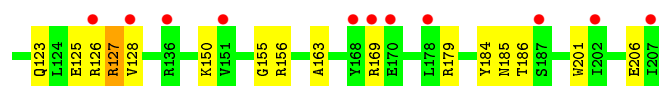


• Molecule 2: 30S ribosomal protein S2

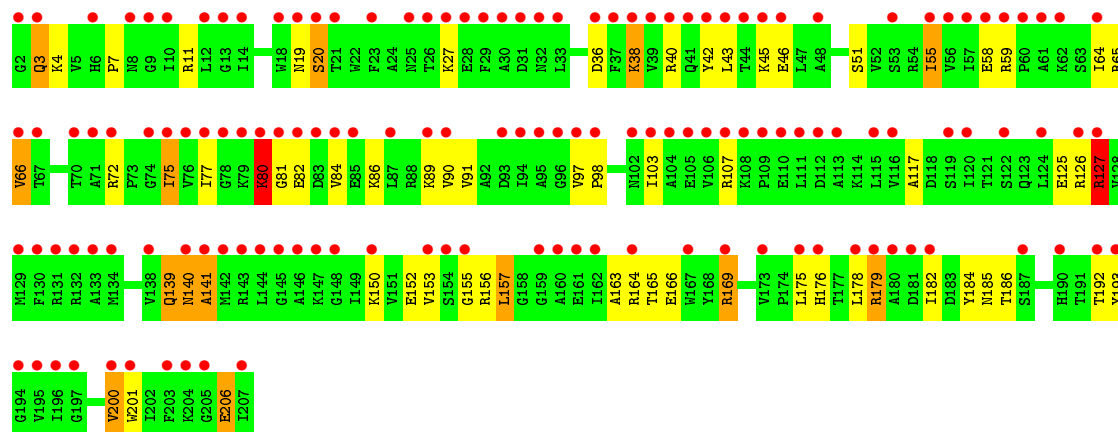


• Molecule 3: 30S ribosomal protein S3

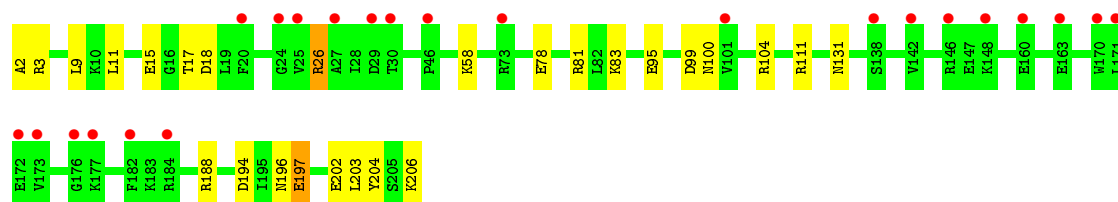
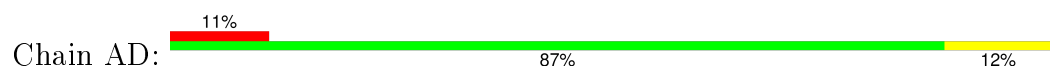




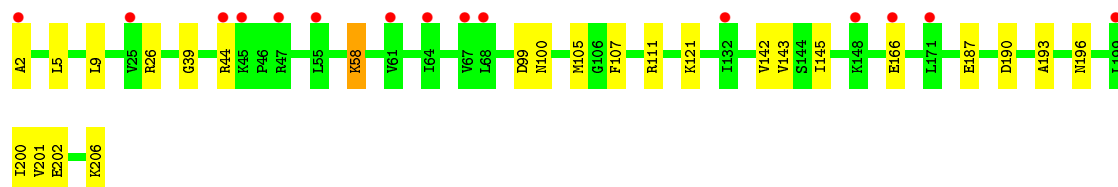
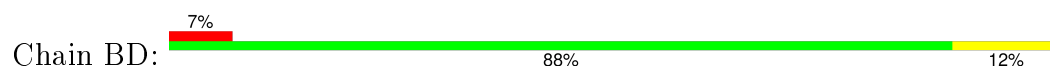
• Molecule 3: 30S ribosomal protein S3



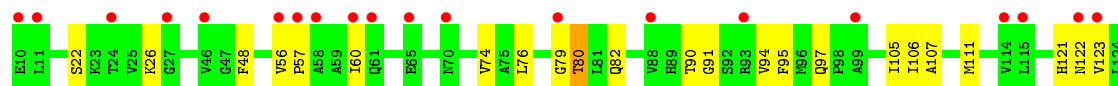
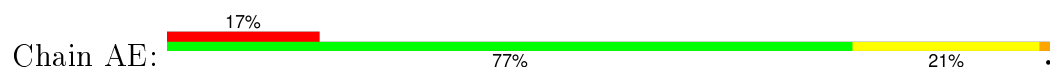
• Molecule 4: 30S ribosomal protein S4

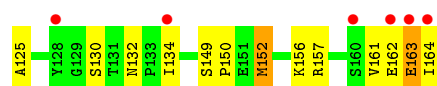


• Molecule 4: 30S ribosomal protein S4

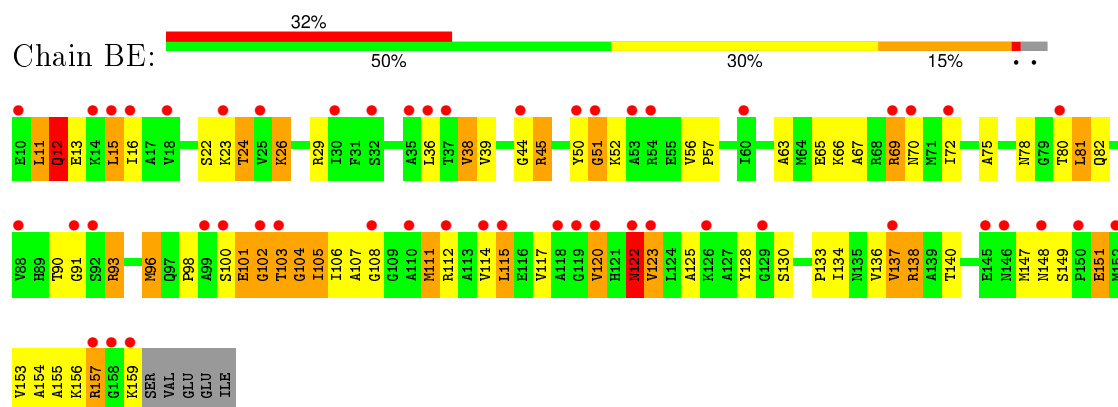


• Molecule 5: 30S ribosomal protein S5

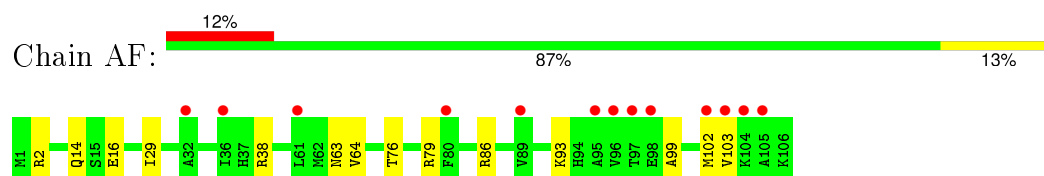




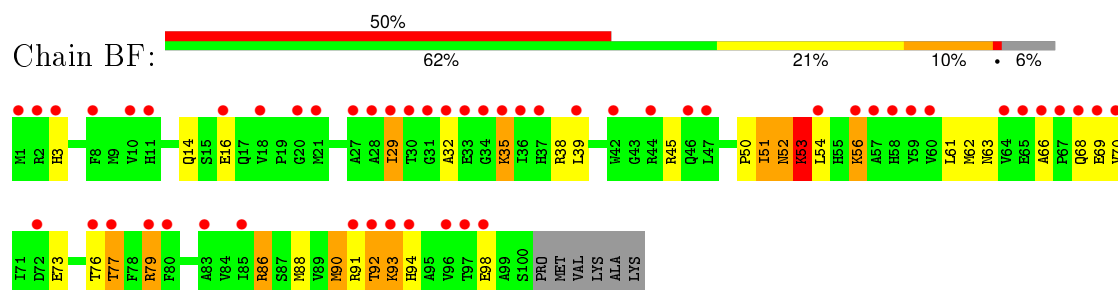
- Molecule 5: 30S ribosomal protein S5



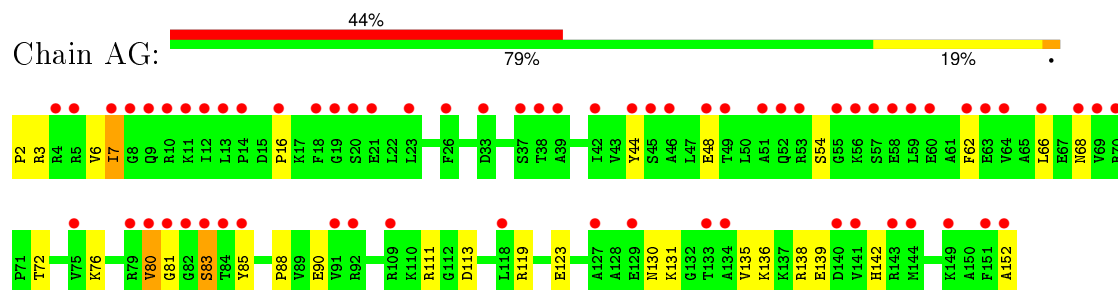
- Molecule 6: 30S ribosomal protein S6



- Molecule 6: 30S ribosomal protein S6

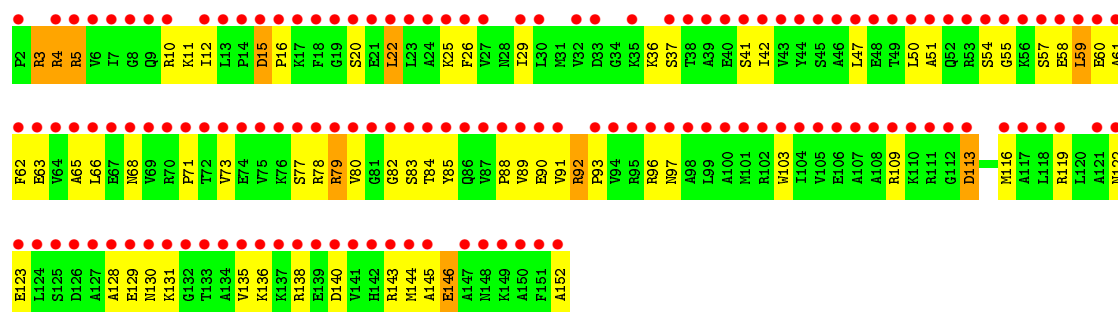


- Molecule 7: 30S ribosomal protein S7

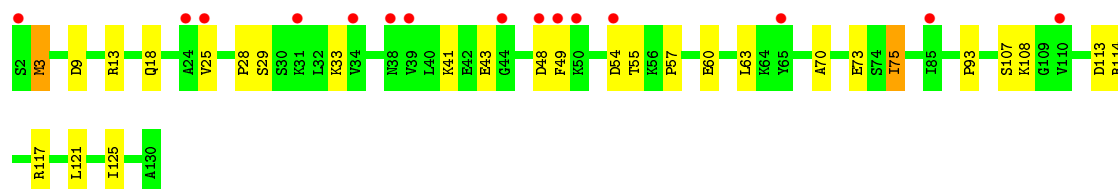
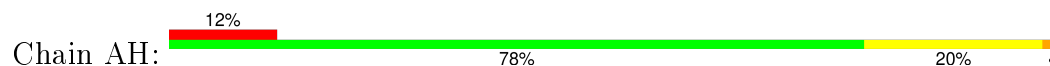


- Molecule 7: 30S ribosomal protein S7

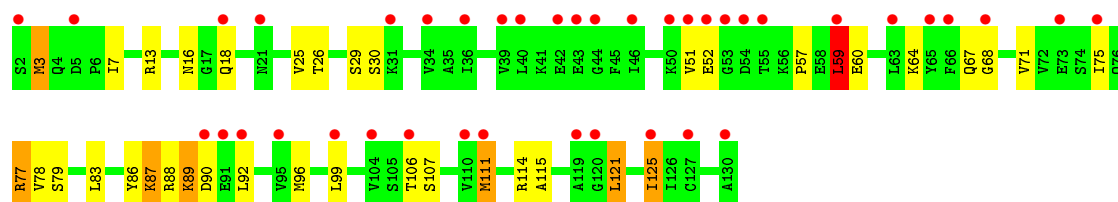
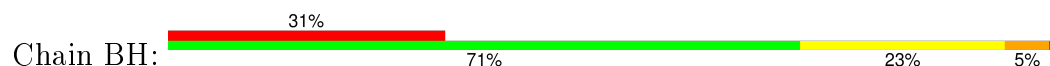




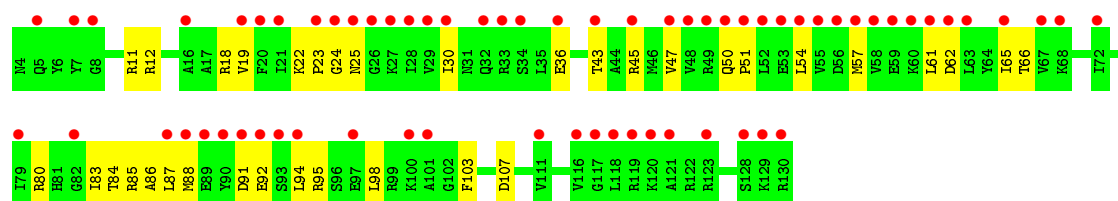
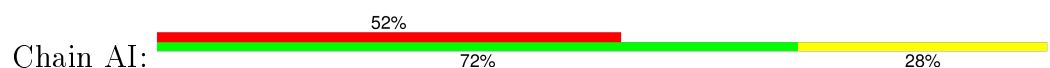
- Molecule 8: 30S ribosomal protein S8



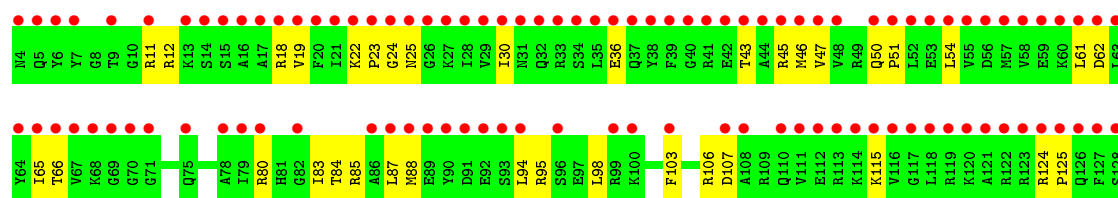
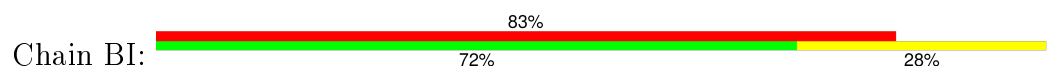
- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9

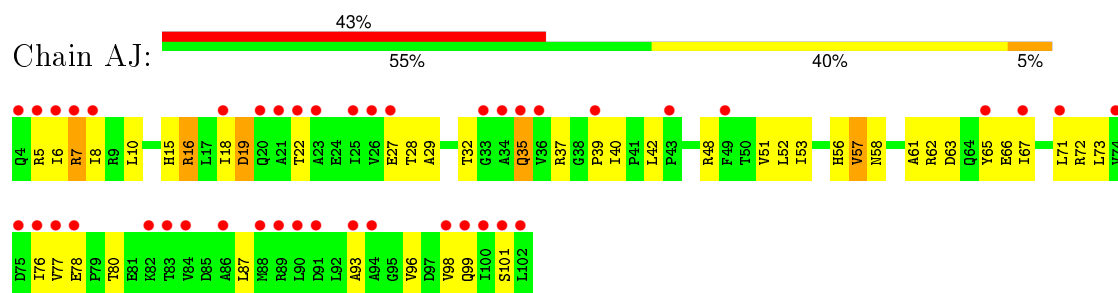


- Molecule 9: 30S ribosomal protein S9

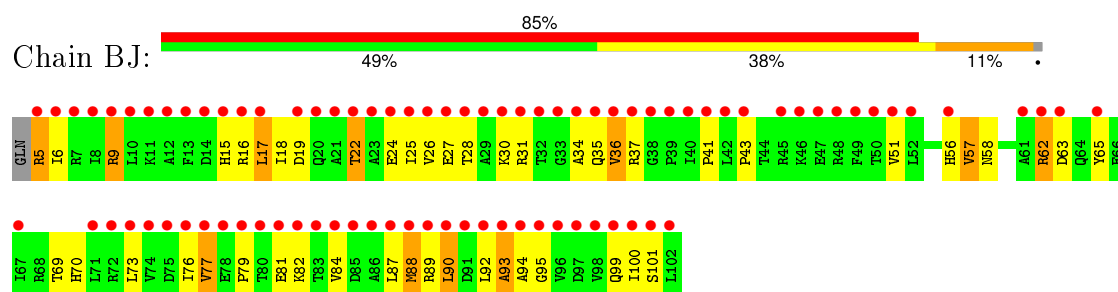




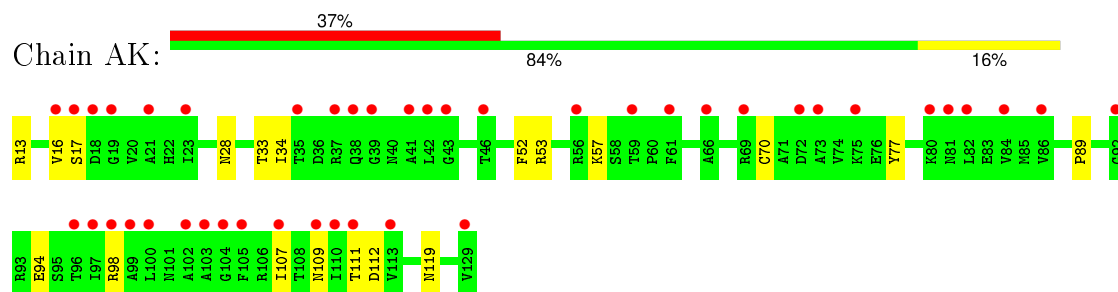
- Molecule 10: 30S ribosomal protein S10



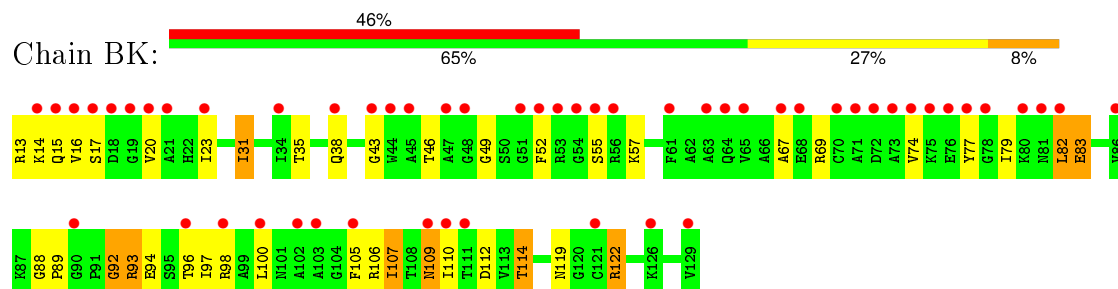
- Molecule 10: 30S ribosomal protein S10



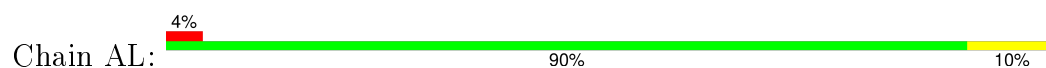
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11

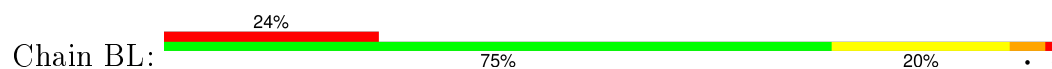


- Molecule 12: 30S ribosomal protein S12

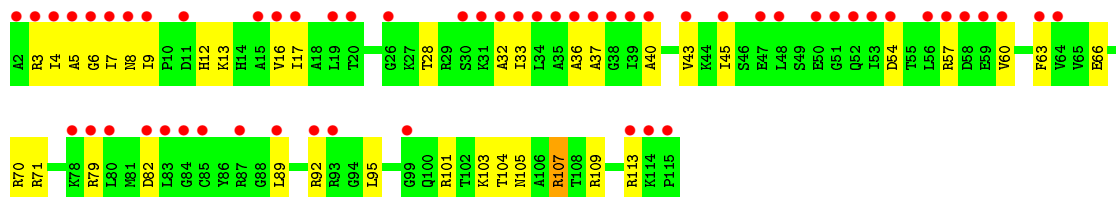




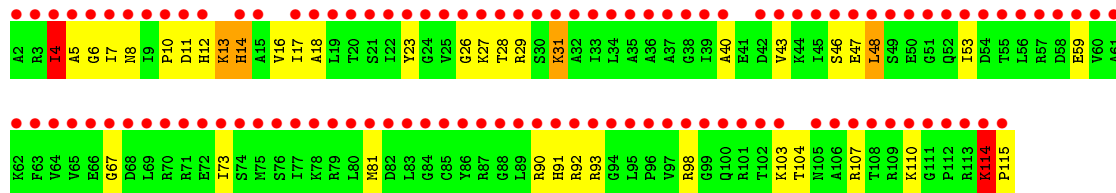
- Molecule 12: 30S ribosomal protein S12



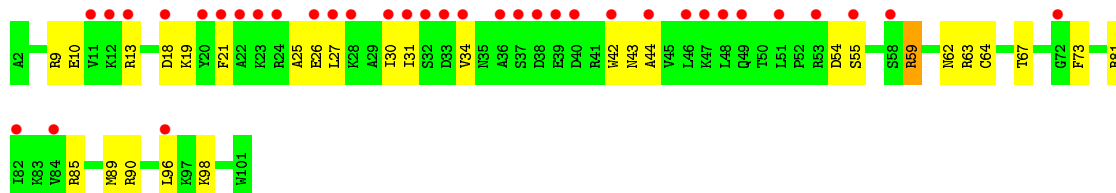
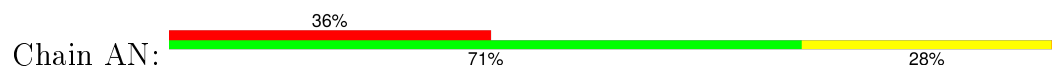
- Molecule 13: 30S ribosomal protein S13



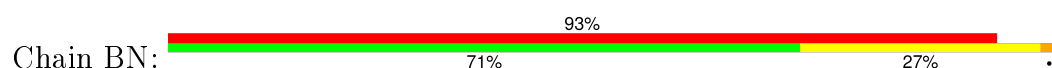
- Molecule 13: 30S ribosomal protein S13

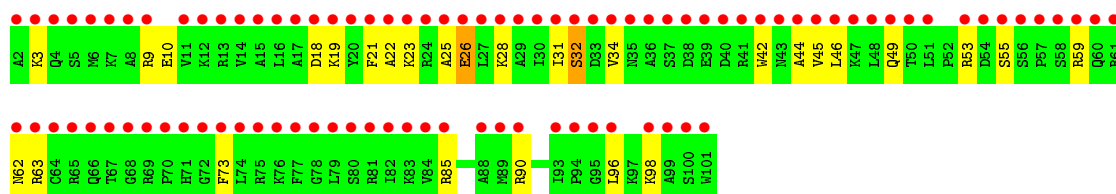


- Molecule 14: 30S ribosomal protein S14

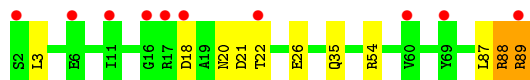
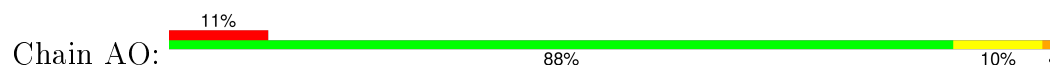


- Molecule 14: 30S ribosomal protein S14

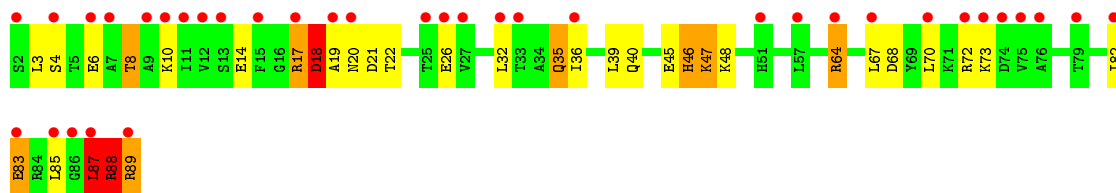
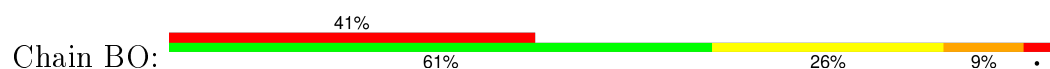




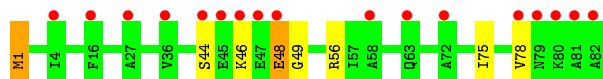
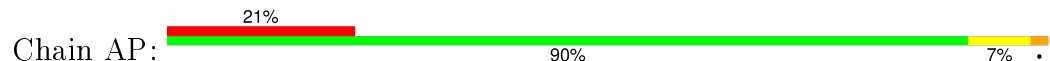
- Molecule 15: 30S ribosomal protein S15



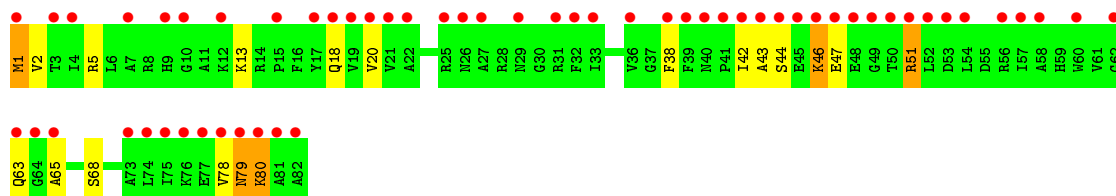
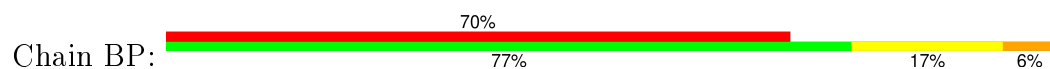
- Molecule 15: 30S ribosomal protein S15



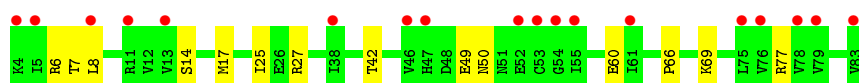
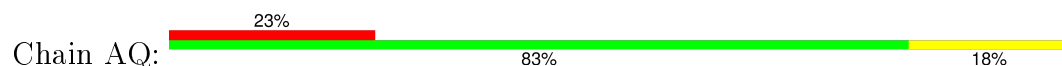
- Molecule 16: 30S ribosomal protein S16



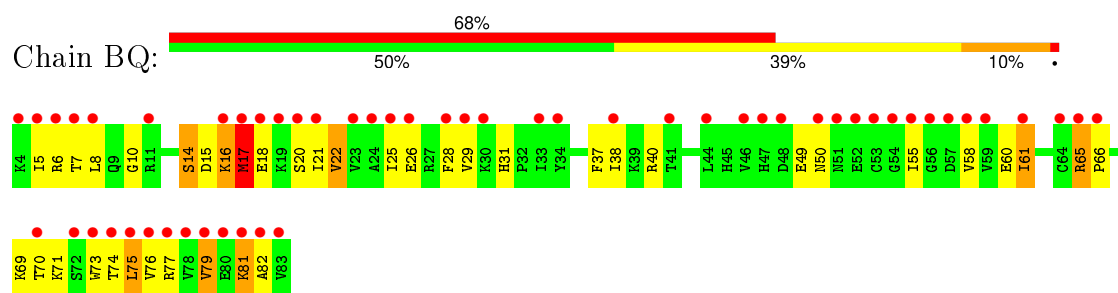
- Molecule 16: 30S ribosomal protein S16



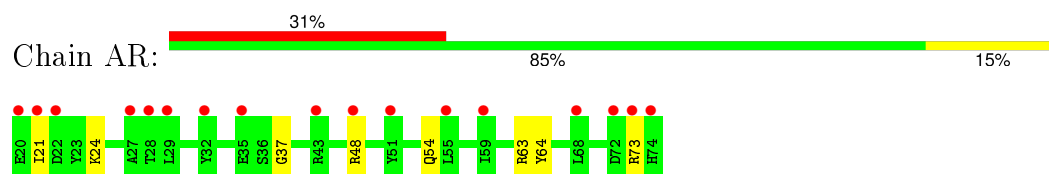
- Molecule 17: 30S ribosomal protein S17



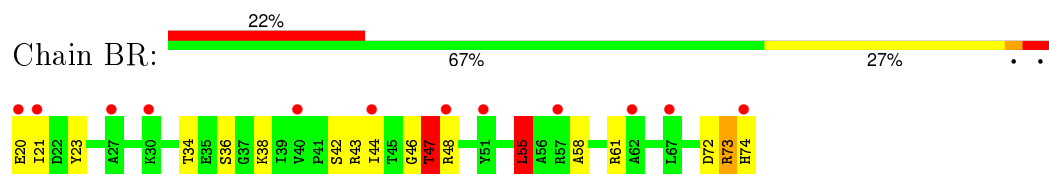
- Molecule 17: 30S ribosomal protein S17



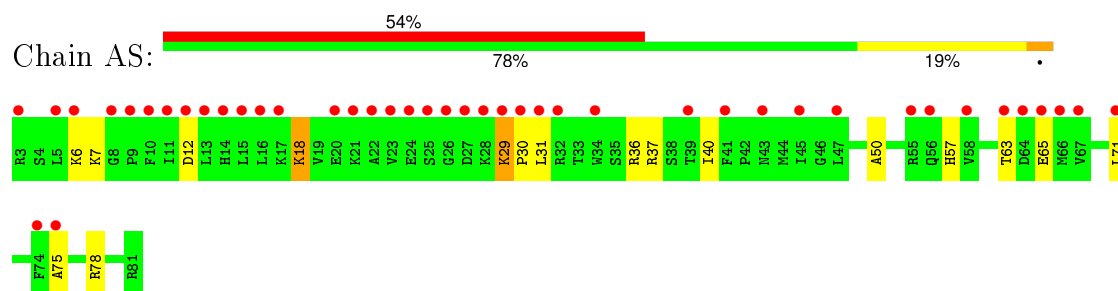
- Molecule 18: 30S ribosomal protein S18



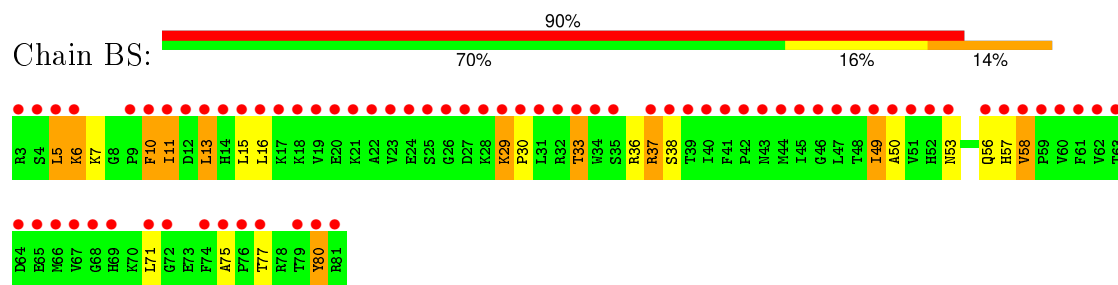
- Molecule 18: 30S ribosomal protein S18



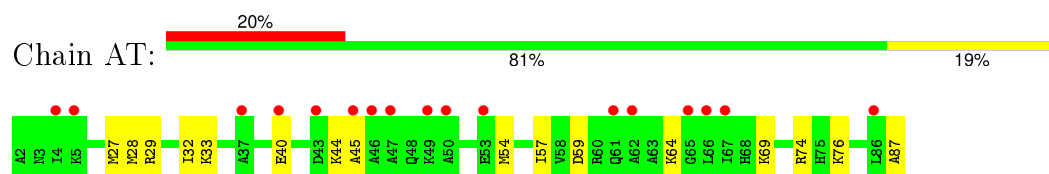
- Molecule 19: 30S ribosomal protein S19



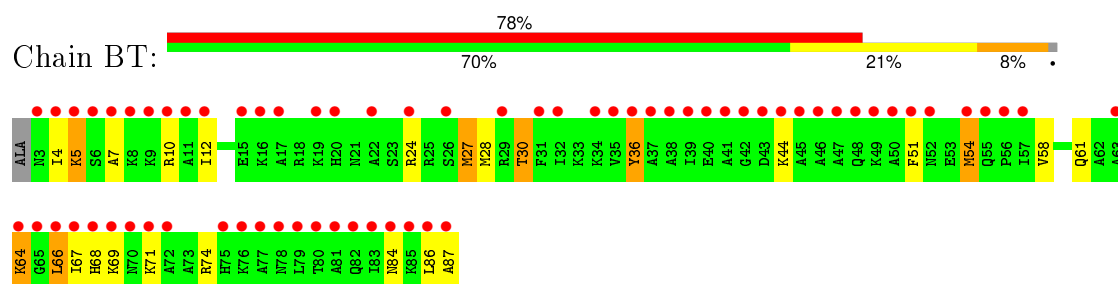
- Molecule 19: 30S ribosomal protein S19



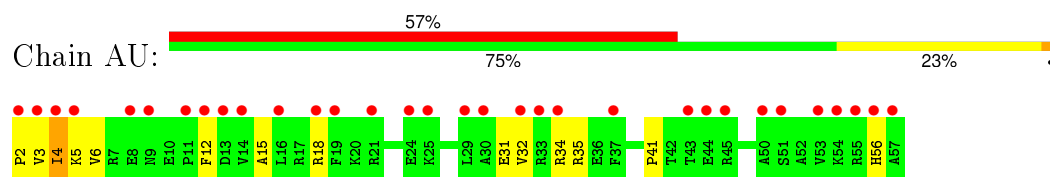
- Molecule 20: 30S ribosomal protein S20



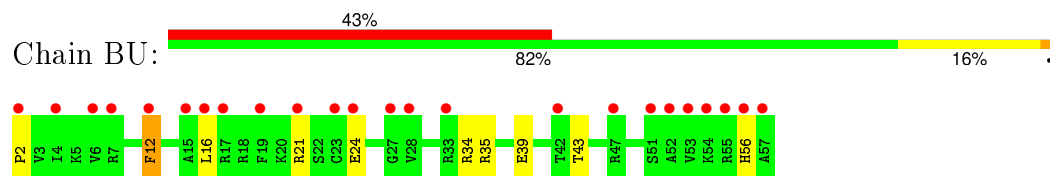
- Molecule 20: 30S ribosomal protein S20



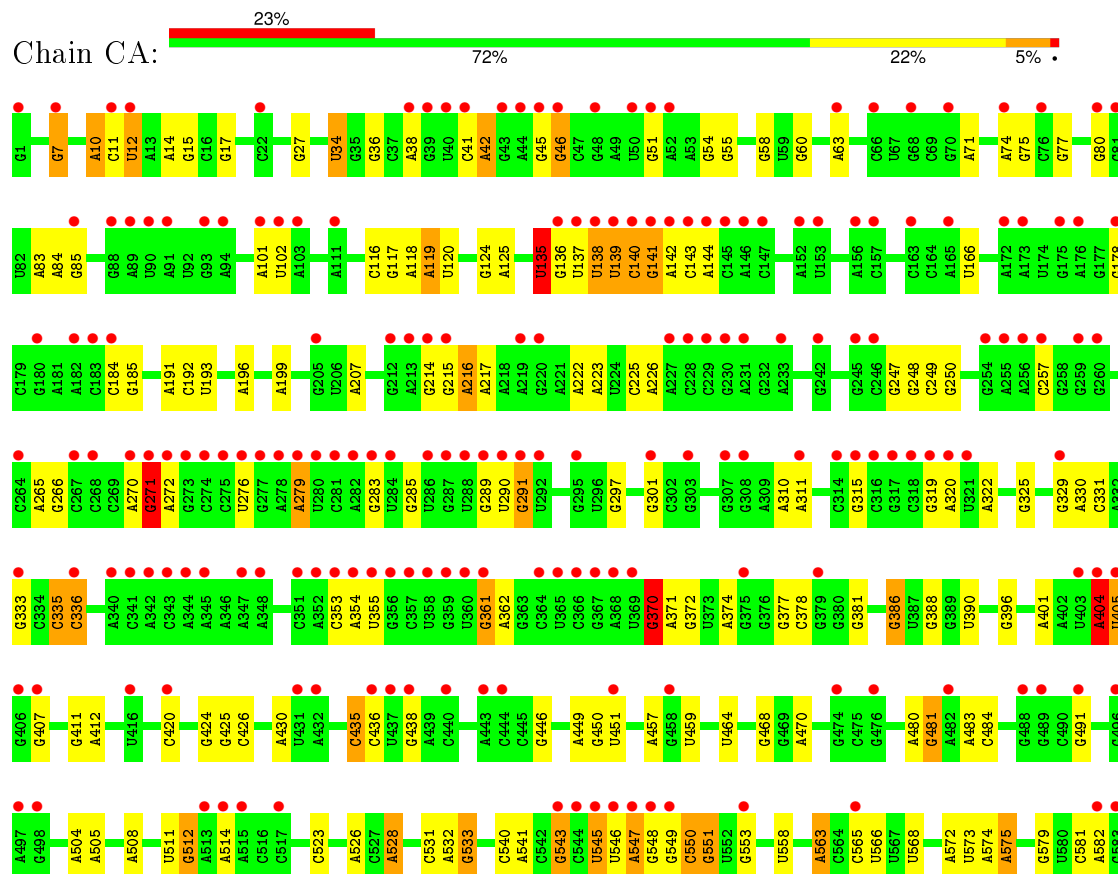
- Molecule 21: 30S ribosomal protein S21



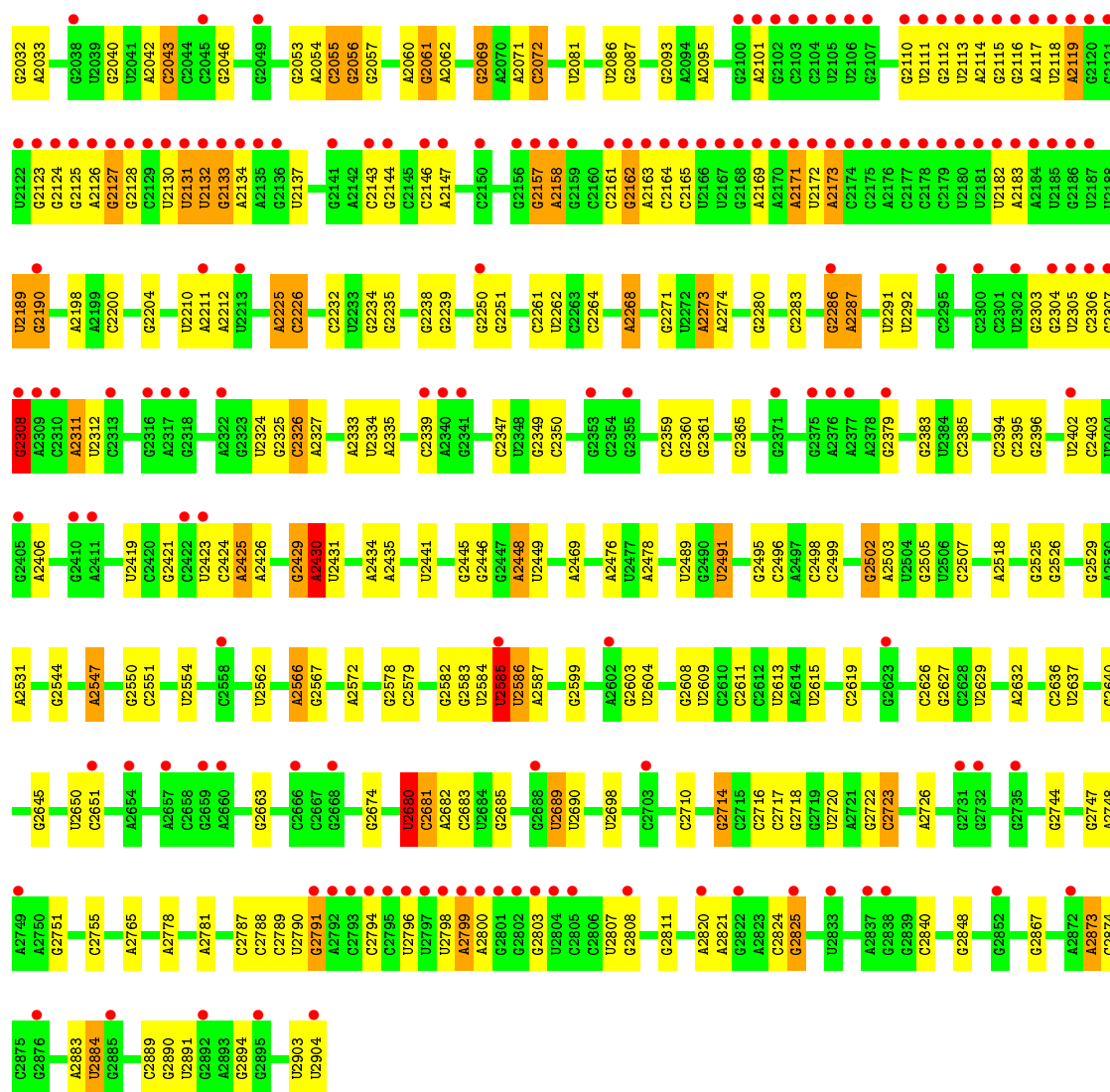
- Molecule 21: 30S ribosomal protein S21



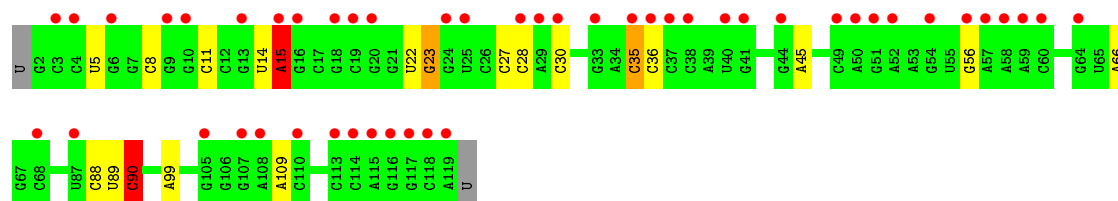
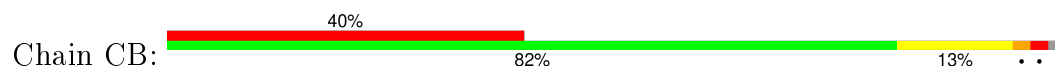
- Molecule 22: 23S rRNA



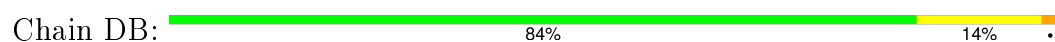




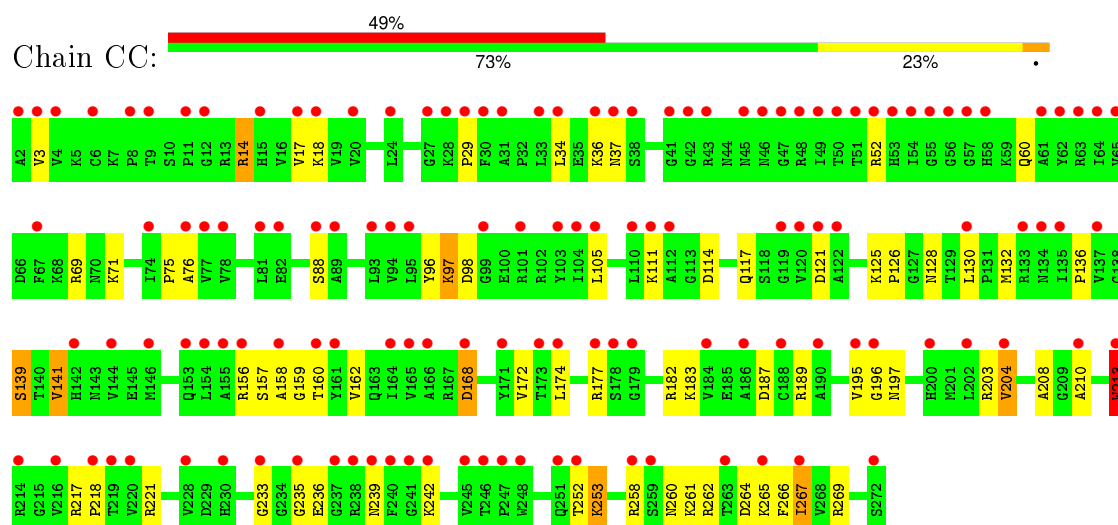
• Molecule 23: 5S rRNA



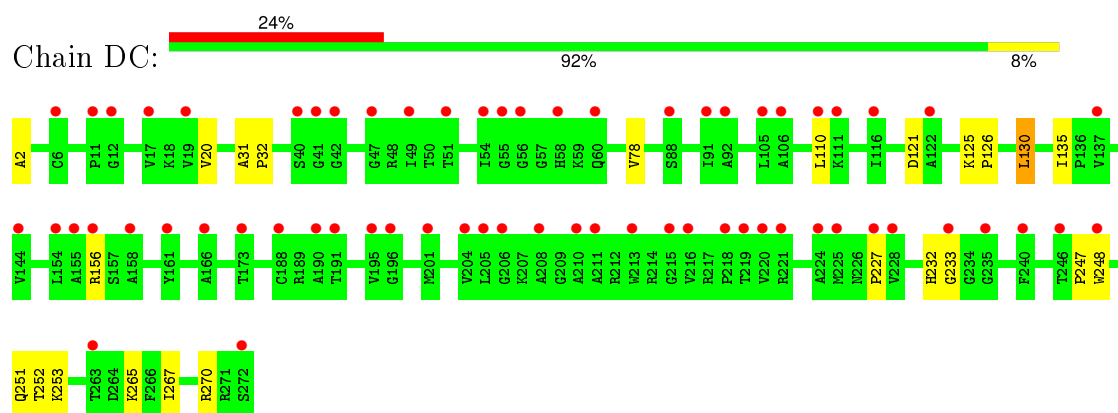
• Molecule 23: 5S rRNA



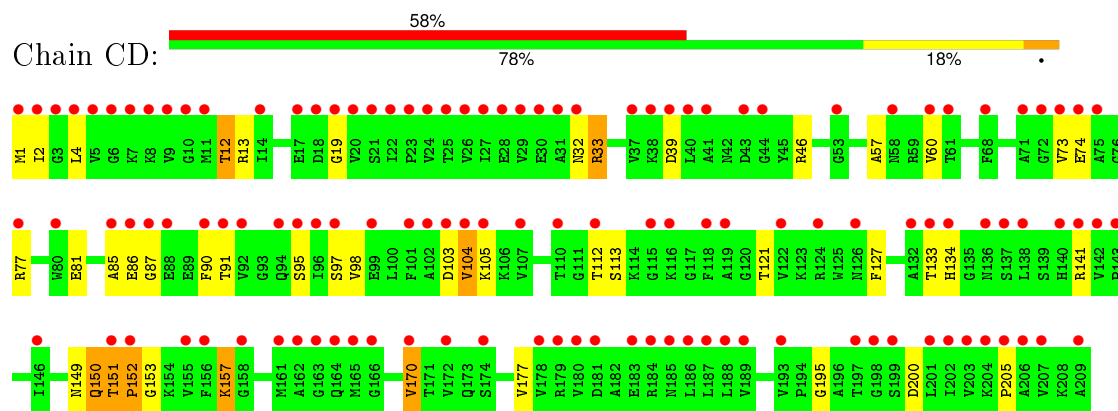
• Molecule 24: 50S ribosomal protein L2



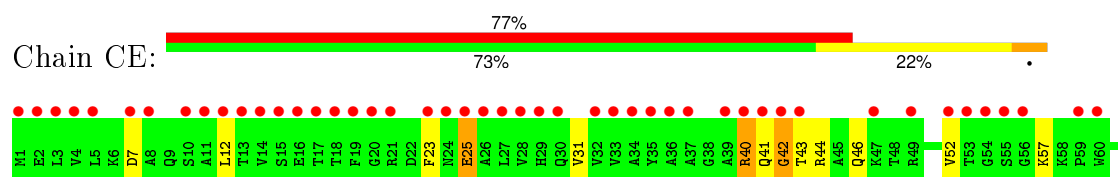
- Molecule 24: 50S ribosomal protein L2

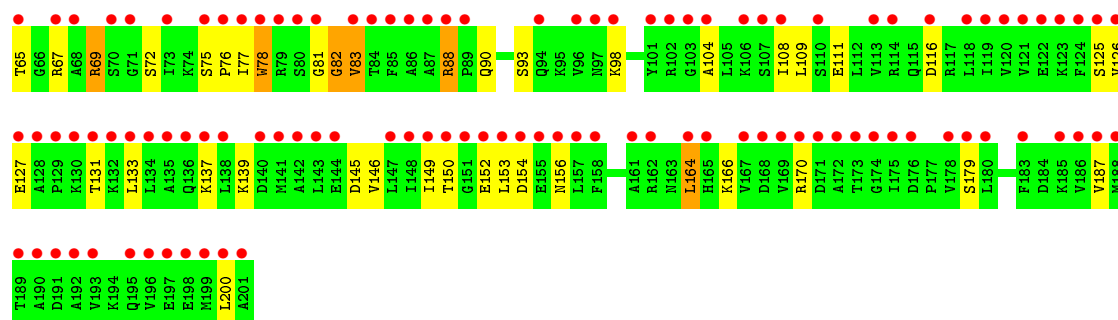


- Molecule 25: 50S ribosomal protein L3

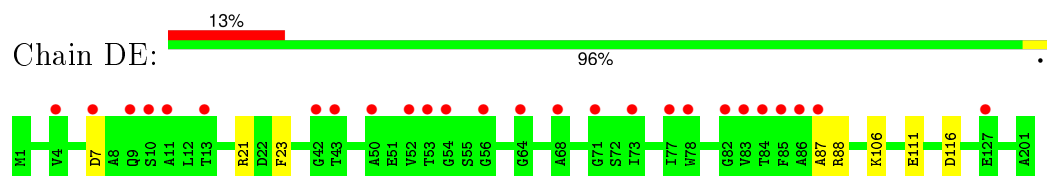


- Molecule 26: 50S ribosomal protein L4

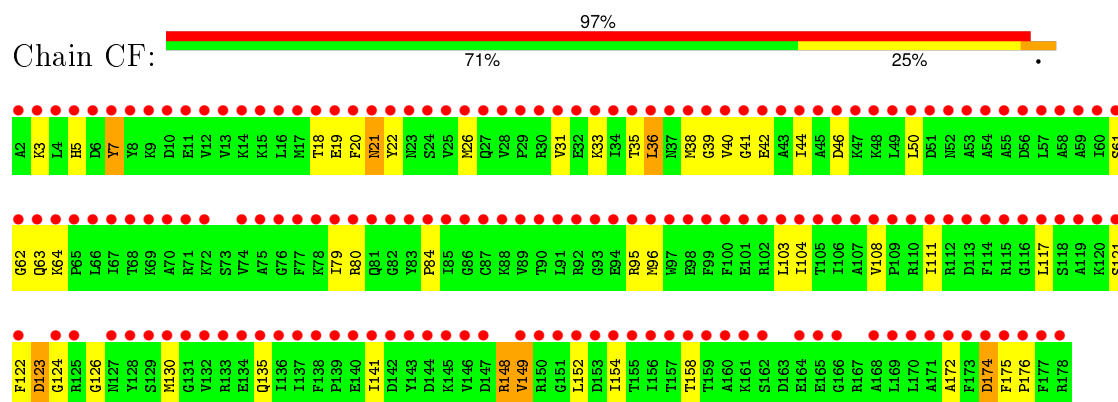


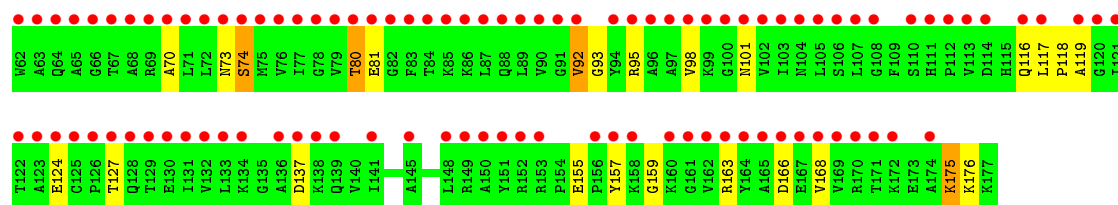


- Molecule 26: 50S ribosomal protein L4

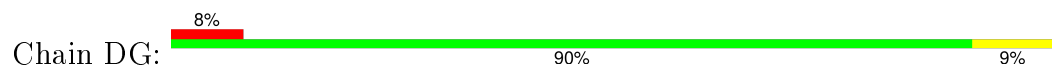


- Molecule 27: 50S ribosomal protein L5

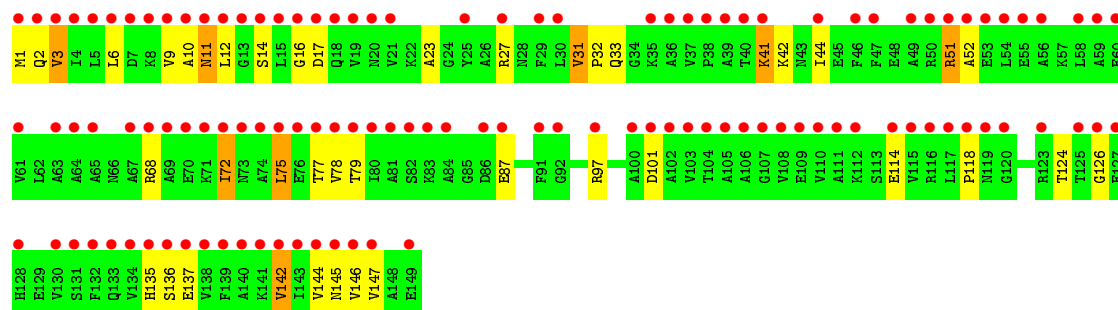
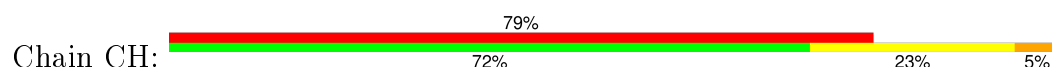




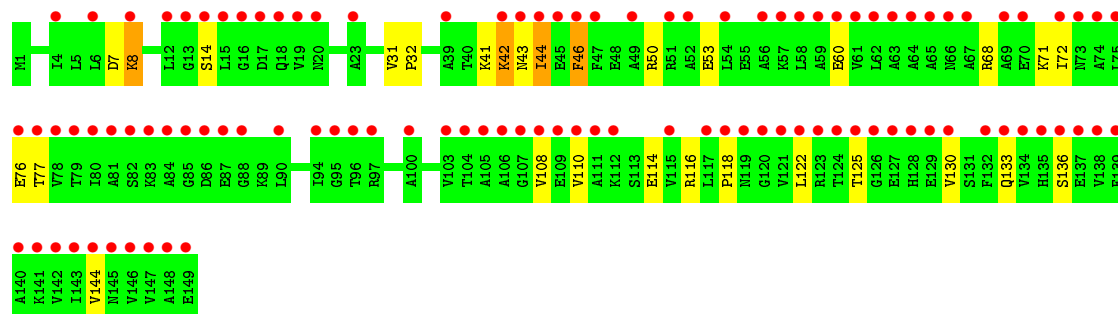
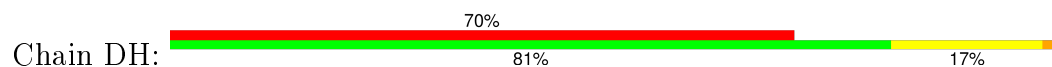
• Molecule 28: 50S ribosomal protein L6



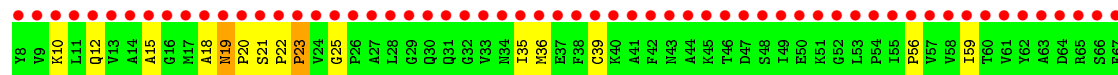
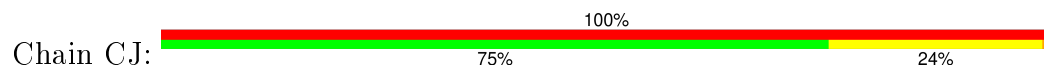
• Molecule 29: 50S ribosomal protein L9

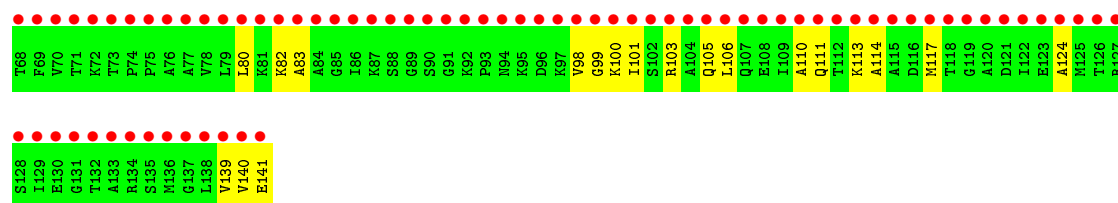


• Molecule 29: 50S ribosomal protein L9



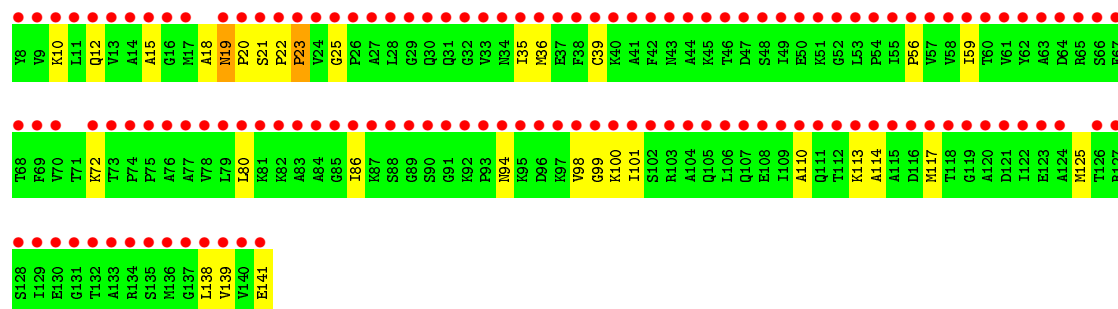
• Molecule 30: 50S ribosomal protein L11





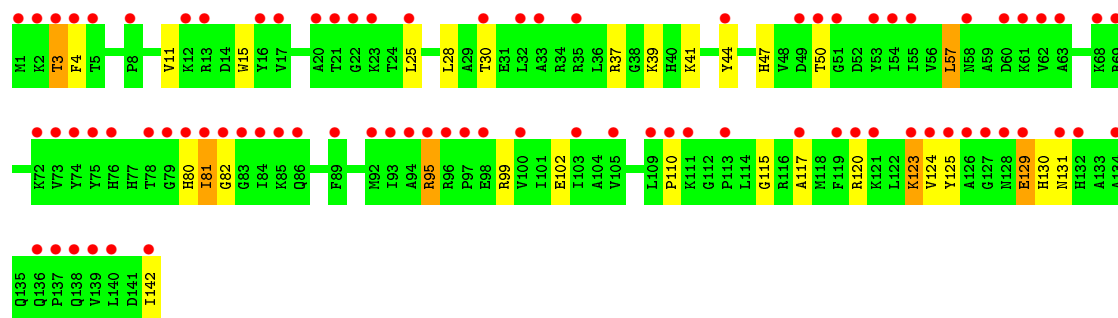
• Molecule 30: 50S ribosomal protein L11

Chain DJ: 98% 77% 22%



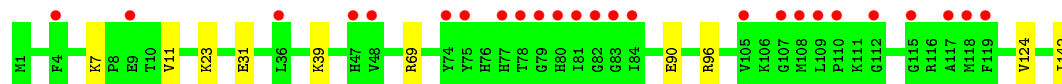
• Molecule 31: 50S ribosomal protein L13

Chain CK: 58% 78% 18%



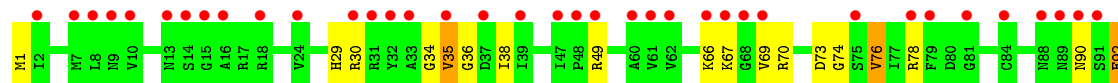
• Molecule 31: 50S ribosomal protein L13

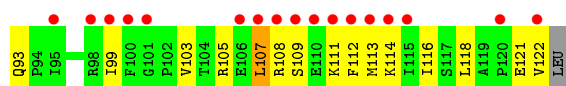
Chain DK: 18% 93% 7%



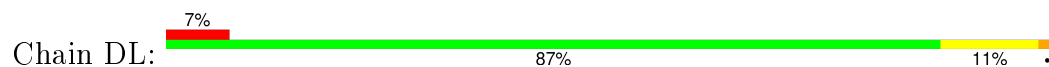
• Molecule 32: 50S ribosomal protein L14

Chain CL: 44% 72% 24%

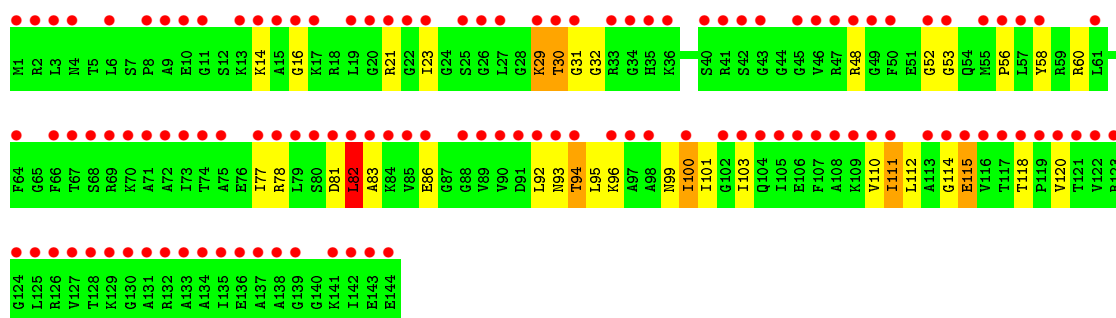
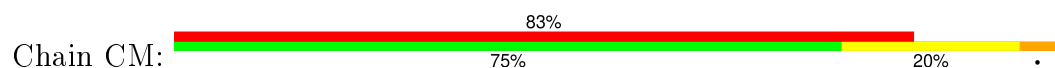




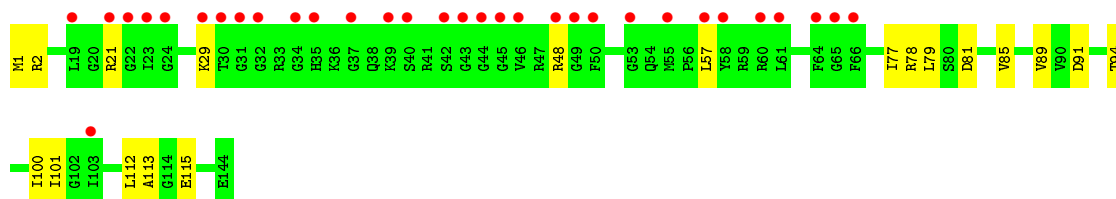
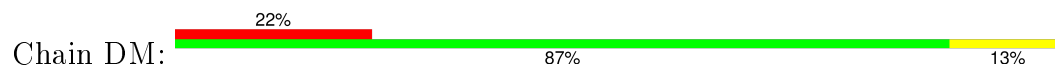
- Molecule 32: 50S ribosomal protein L14



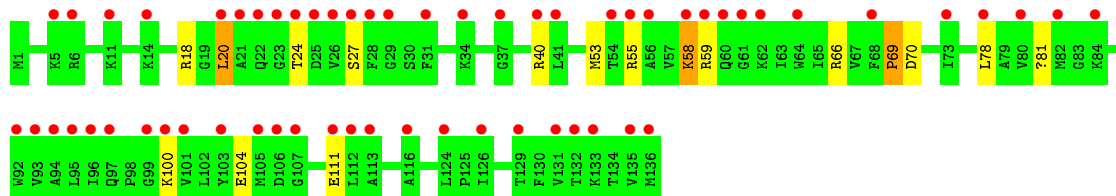
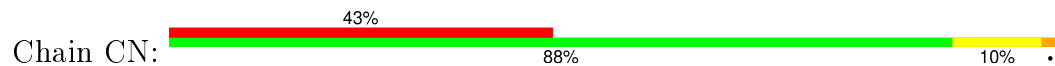
- Molecule 33: 50S ribosomal protein L15



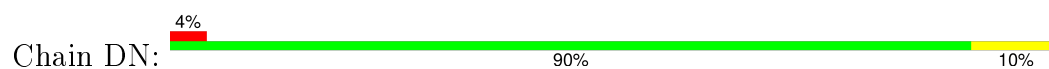
- Molecule 33: 50S ribosomal protein L15

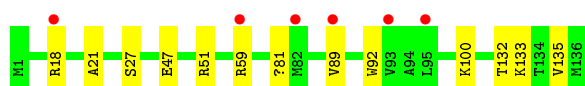


- Molecule 34: 50S ribosomal protein L16

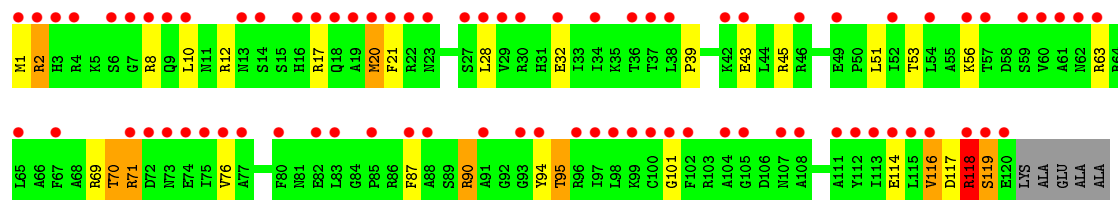
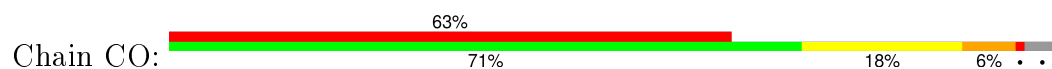


- Molecule 34: 50S ribosomal protein L16

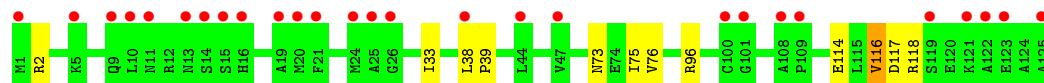
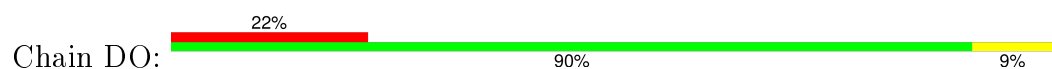




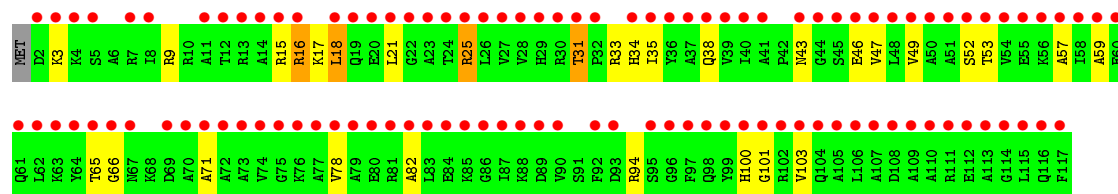
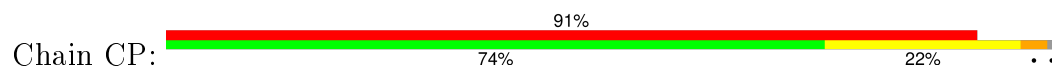
- Molecule 35: 50S ribosomal protein L17



- Molecule 35: 50S ribosomal protein L17



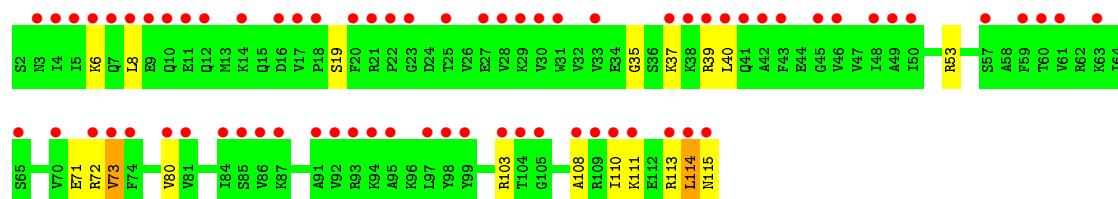
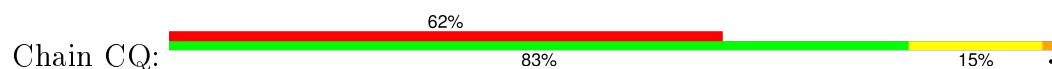
- Molecule 36: 50S ribosomal protein L18



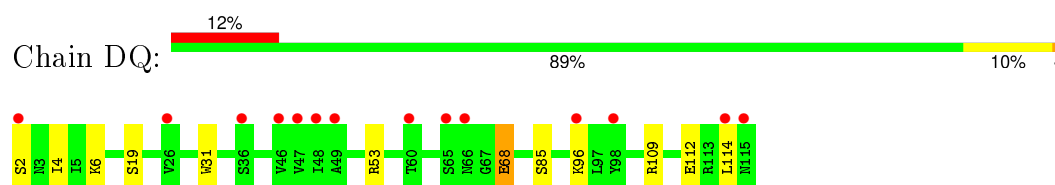
- Molecule 36: 50S ribosomal protein L18



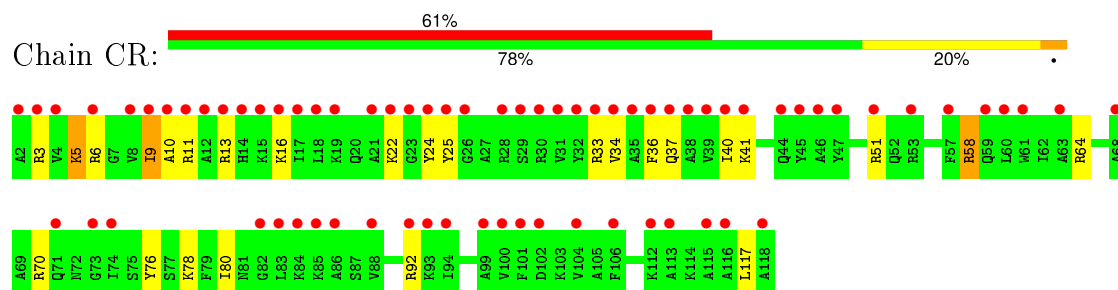
- Molecule 37: 50S ribosomal protein L19



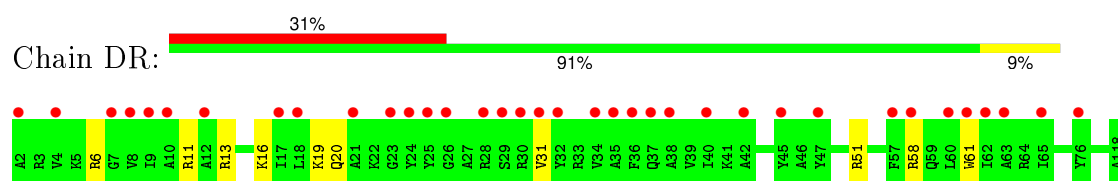
- Molecule 37: 50S ribosomal protein L19



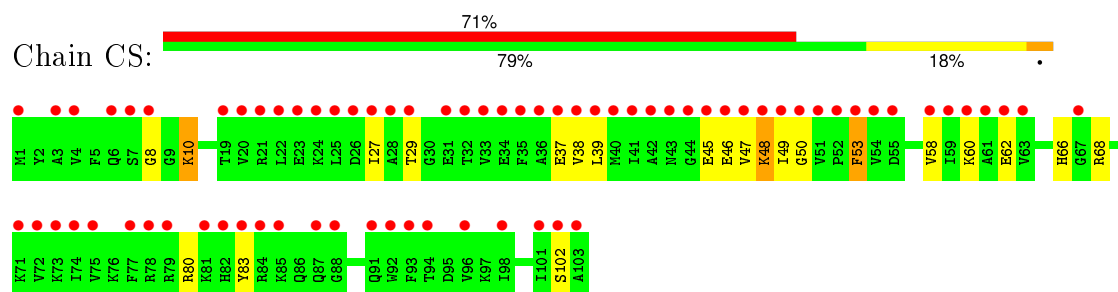
• Molecule 38: 50S ribosomal protein L20



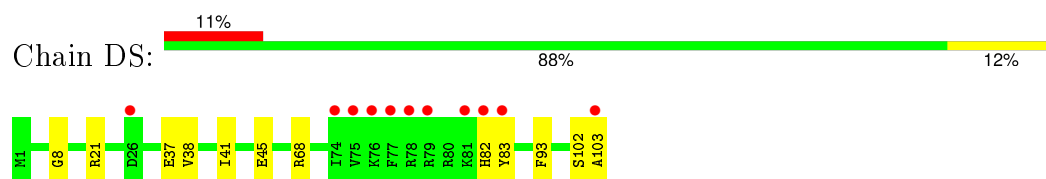
• Molecule 38: 50S ribosomal protein L20



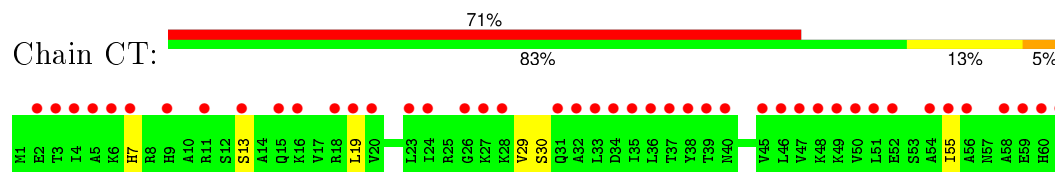
• Molecule 39: 50S ribosomal protein L21

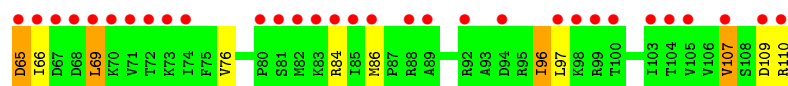


• Molecule 39: 50S ribosomal protein L21

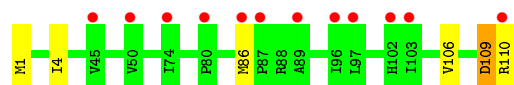


• Molecule 40: 50S ribosomal protein L22

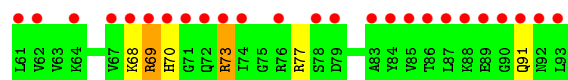
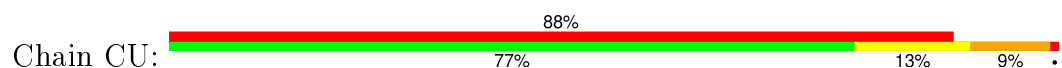




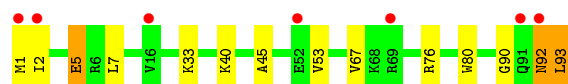
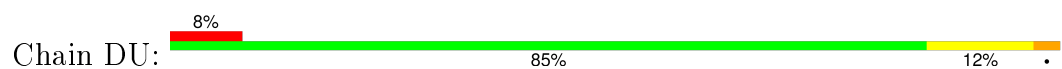
- Molecule 40: 50S ribosomal protein L22



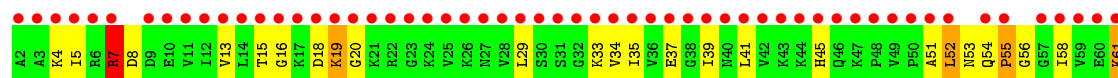
- Molecule 41: 50S ribosomal protein L23



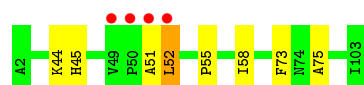
- Molecule 41: 50S ribosomal protein L23



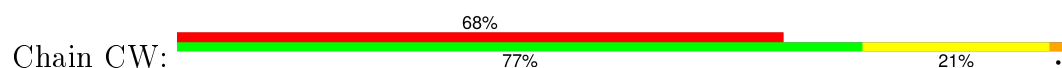
- Molecule 42: 50S ribosomal protein L24

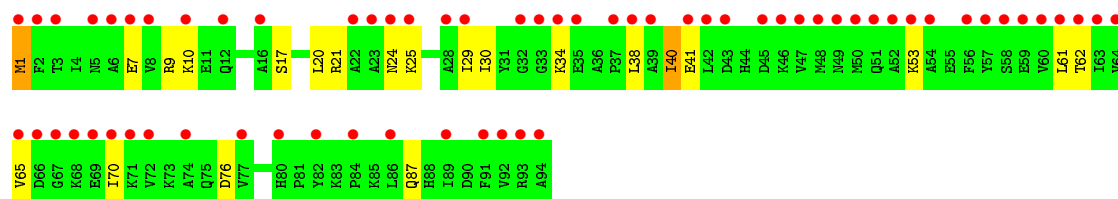


- Molecule 42: 50S ribosomal protein L24

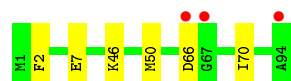


- Molecule 43: 50S ribosomal protein L25

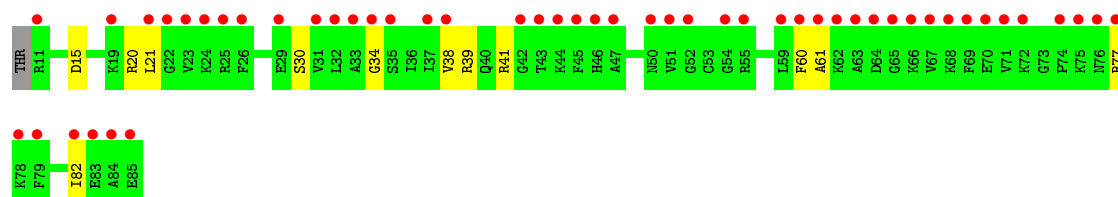
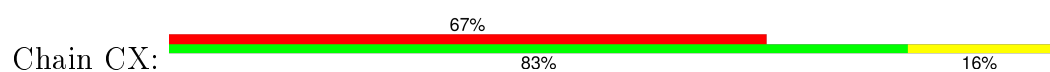




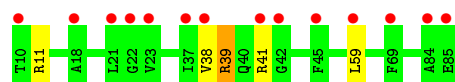
- Molecule 43: 50S ribosomal protein L25



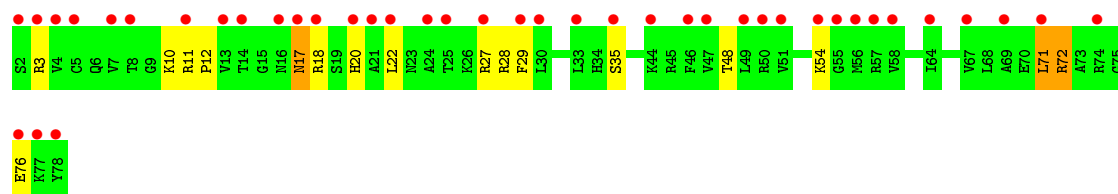
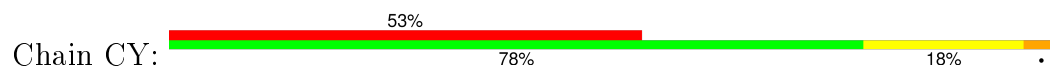
- Molecule 44: 50S ribosomal protein L27



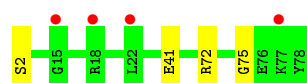
- Molecule 44: 50S ribosomal protein L27



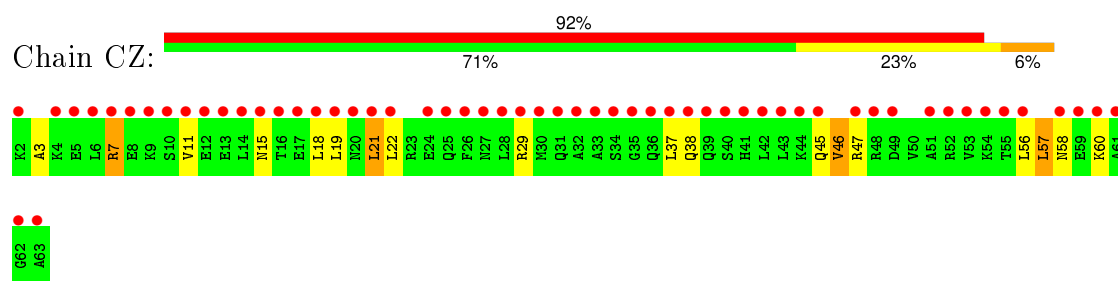
- Molecule 45: 50S ribosomal protein L28



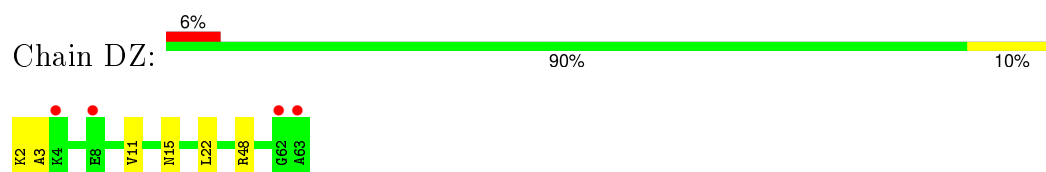
- Molecule 45: 50S ribosomal protein L28



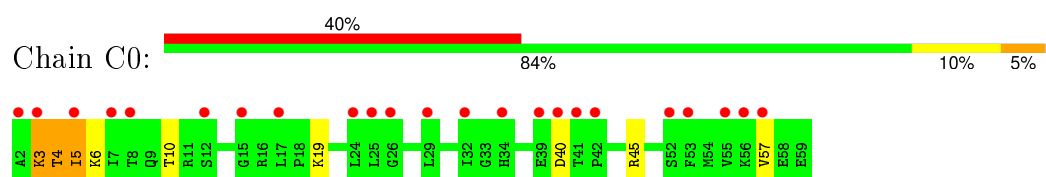
- Molecule 46: 50S ribosomal protein L29



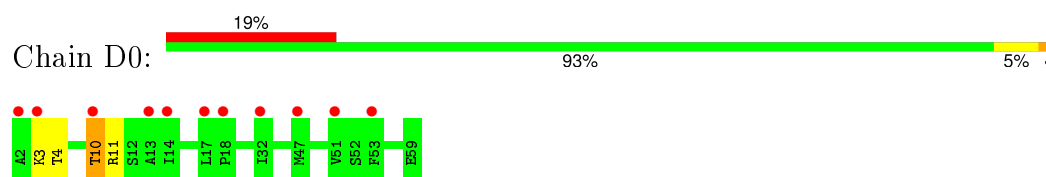
- Molecule 46: 50S ribosomal protein L29



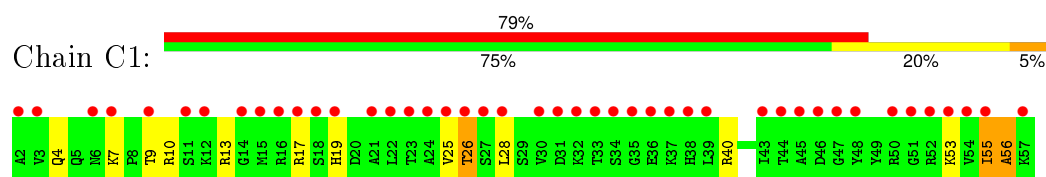
- Molecule 47: 50S ribosomal protein L30



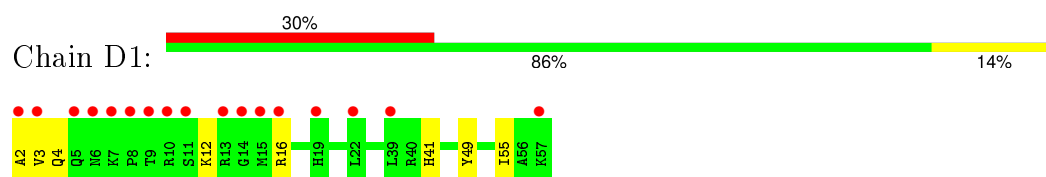
- Molecule 47: 50S ribosomal protein L30



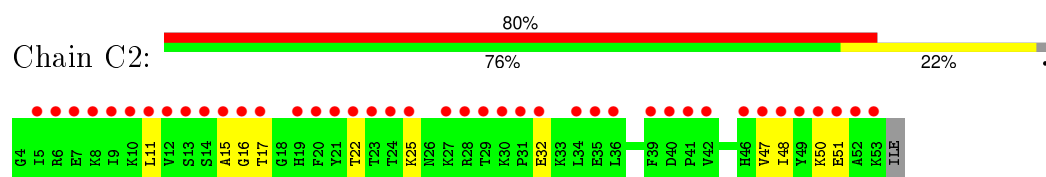
- Molecule 48: 50S ribosomal protein L32



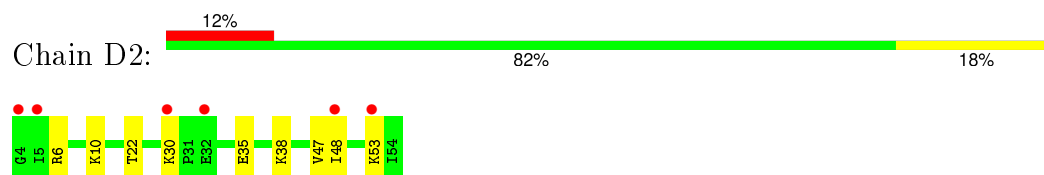
- Molecule 48: 50S ribosomal protein L32



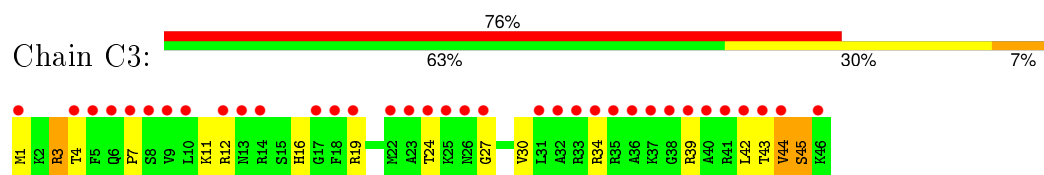
- Molecule 49: 50S ribosomal protein L33



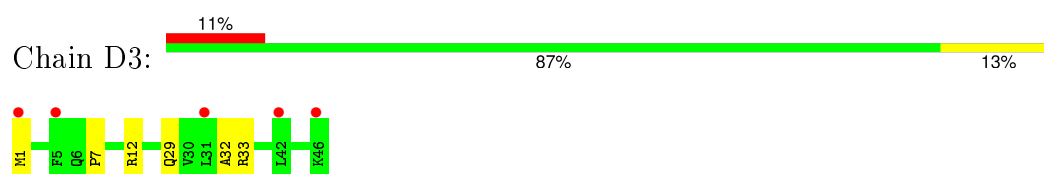
- Molecule 49: 50S ribosomal protein L33



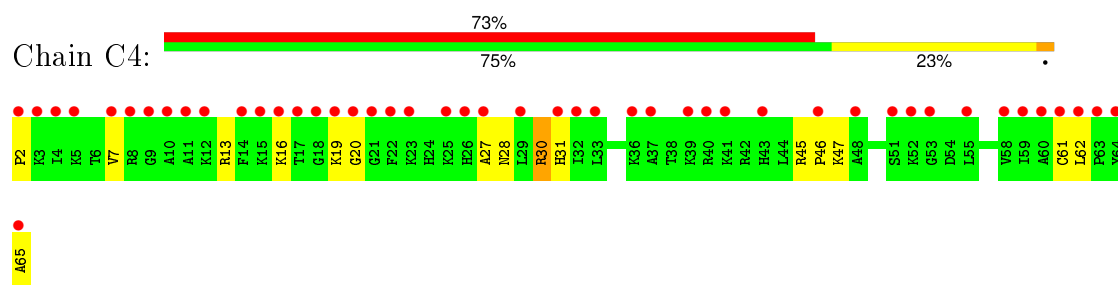
- Molecule 50: 50S ribosomal protein L34



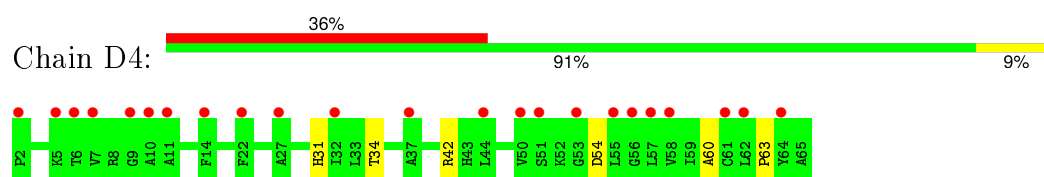
- Molecule 50: 50S ribosomal protein L34



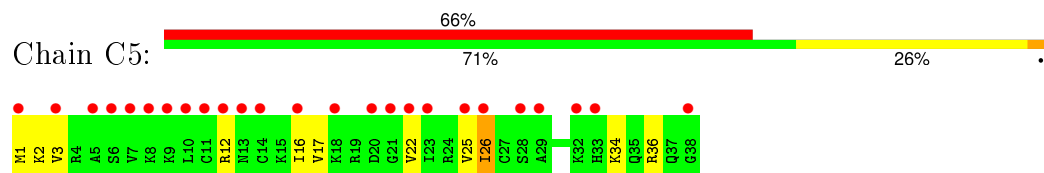
- Molecule 51: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L35

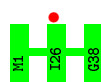


- Molecule 52: 50S ribosomal protein L36

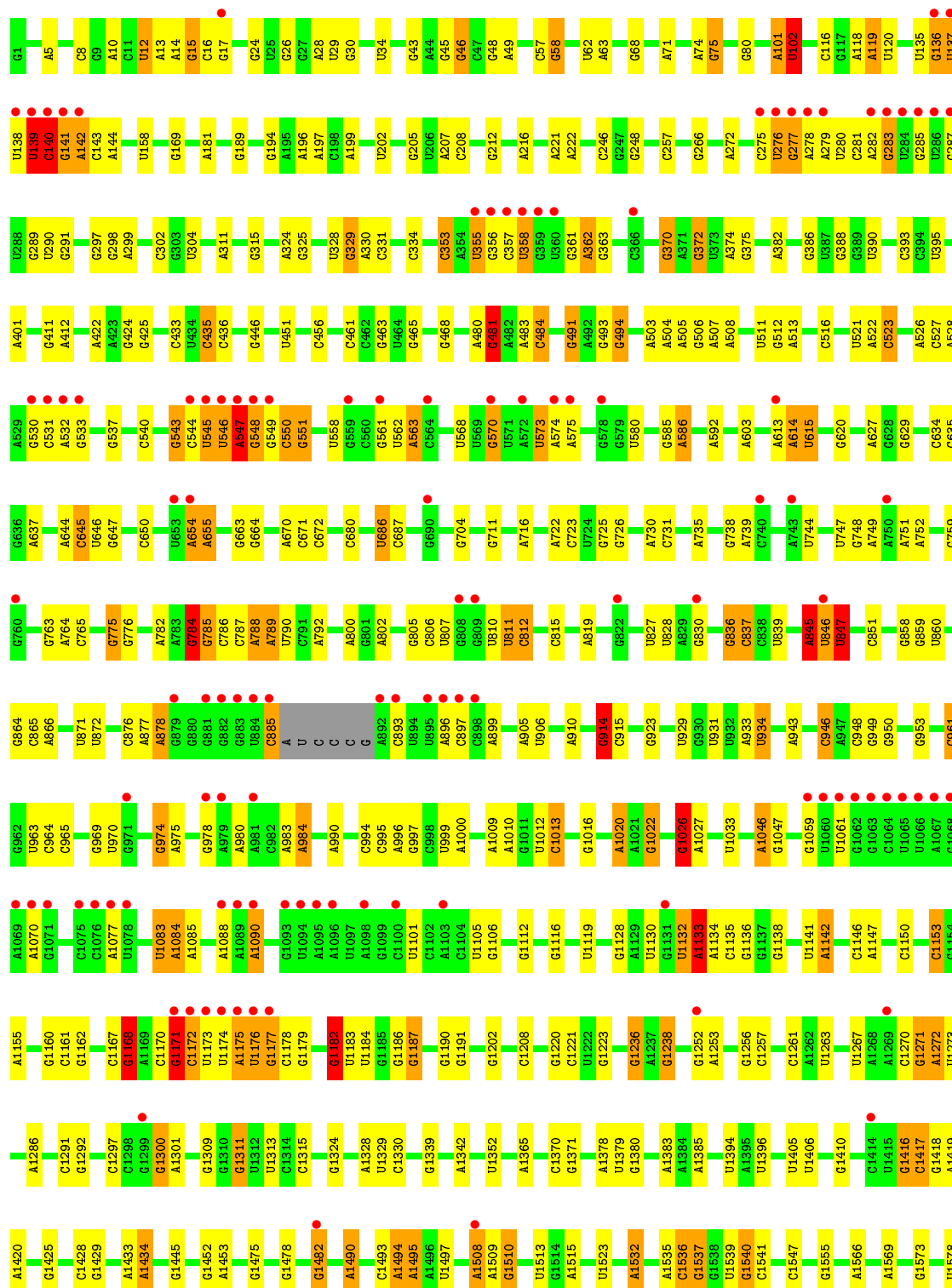


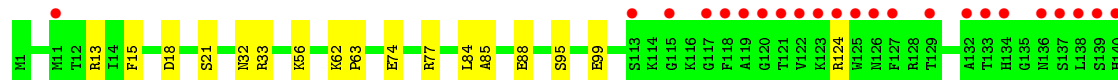
- Molecule 52: 50S ribosomal protein L36

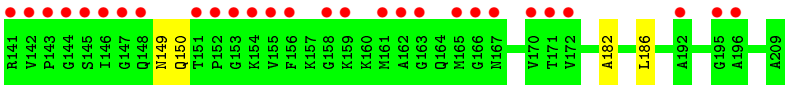




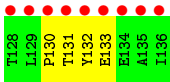
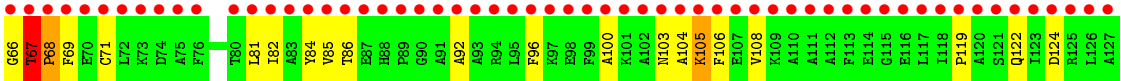
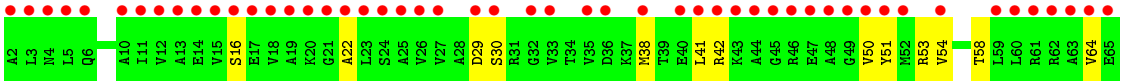
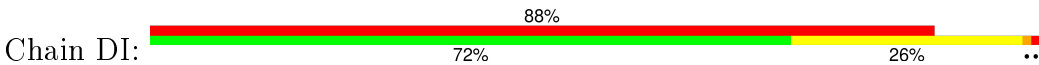
• Molecule 53: 23S rRNA







● Molecule 55: 50S ribosomal protein L10



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 212.17Å 433.89Å 624.25Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 69.39 – 2.10 69.39 – 2.10 | Depositor EDS |
| % Data completeness (in resolution range) | 93.0 (69.39-2.10) 93.0 (69.39-2.10) | Depositor EDS |
| R_{merge} | 0.15 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 0.99 (at 2.10Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | 0.218 , 0.234 0.242 , 0.258 | Depositor DCC |
| R_{free} test set | 10048 reflections (0.33%) | DCC |
| Wilson B-factor (Å ²) | 52.5 | Xtriage |
| Anisotropy | 0.173 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 51.8 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Outliers | 0 of 3063926 reflections | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 295060 | wwPDB-VP |
| Average B, all atoms (Å ²) | 94.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, GUN, 1PE, 2MA, 2MG, ACY, PEG, 1MG, 3TD, PGE, G7M, D2T, UR3, SPD, 4D4, 5MU, ZN, 5MC, MPD, PG4, 6MZ, TRS, OMC, MG, OMG, H2U, EDO, MEQ, OMU, PUT, 4OC, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | AA | 0.58 | 0/36593 | 0.98 | 33/57081 (0.1%) |
| 1 | BA | 0.52 | 0/36568 | 1.03 | 90/57042 (0.2%) |
| 2 | AB | 0.36 | 0/1784 | 0.55 | 0/2403 |
| 2 | BB | 0.39 | 0/1784 | 0.59 | 0/2403 |
| 3 | AC | 0.39 | 0/1652 | 0.55 | 0/2225 |
| 3 | BC | 0.42 | 0/1652 | 0.76 | 0/2225 |
| 4 | AD | 0.37 | 0/1665 | 0.53 | 0/2227 |
| 4 | BD | 0.43 | 0/1665 | 0.57 | 0/2227 |
| 5 | AE | 0.48 | 0/1157 | 0.61 | 0/1557 |
| 5 | BE | 0.56 | 0/1118 | 1.07 | 4/1504 (0.3%) |
| 6 | AF | 0.43 | 0/881 | 0.56 | 0/1189 |
| 6 | BF | 0.47 | 0/835 | 0.90 | 2/1128 (0.2%) |
| 7 | AG | 0.35 | 0/1196 | 0.51 | 0/1602 |
| 7 | BG | 0.41 | 0/1196 | 0.83 | 1/1602 (0.1%) |
| 8 | AH | 0.43 | 0/989 | 0.58 | 0/1326 |
| 8 | BH | 0.38 | 0/989 | 0.82 | 3/1326 (0.2%) |
| 9 | AI | 0.37 | 0/1034 | 0.60 | 0/1375 |
| 9 | BI | 0.33 | 0/1034 | 0.60 | 0/1375 |
| 10 | AJ | 0.57 | 0/806 | 0.68 | 0/1089 |
| 10 | BJ | 0.73 | 0/797 | 0.66 | 0/1077 |
| 11 | AK | 0.39 | 0/893 | 0.54 | 0/1205 |
| 11 | BK | 0.45 | 0/893 | 0.86 | 0/1205 |
| 12 | AL | 0.49 | 0/960 | 0.65 | 0/1286 |
| 12 | BL | 0.53 | 0/960 | 0.93 | 3/1286 (0.2%) |
| 13 | AM | 0.38 | 0/893 | 0.63 | 0/1193 |
| 13 | BM | 0.35 | 0/893 | 0.90 | 0/1193 |
| 14 | AN | 0.40 | 0/817 | 0.60 | 0/1088 |
| 14 | BN | 0.49 | 0/817 | 0.70 | 0/1088 |
| 15 | AO | 0.42 | 0/722 | 0.52 | 0/964 |
| 15 | BO | 0.43 | 0/722 | 0.88 | 1/964 (0.1%) |
| 16 | AP | 0.40 | 0/659 | 0.59 | 0/884 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 16 | BP | 0.48 | 0/659 | 0.89 | 0/884 |
| 17 | AQ | 0.44 | 0/658 | 0.61 | 0/881 |
| 17 | BQ | 0.43 | 0/658 | 0.82 | 0/881 |
| 18 | AR | 0.41 | 0/463 | 0.55 | 0/621 |
| 18 | BR | 0.45 | 0/463 | 0.98 | 1/621 (0.2%) |
| 19 | AS | 0.37 | 0/653 | 0.56 | 0/877 |
| 19 | BS | 0.43 | 0/653 | 0.85 | 1/877 (0.1%) |
| 20 | AT | 0.40 | 0/676 | 0.53 | 0/895 |
| 20 | BT | 0.40 | 0/671 | 0.82 | 1/888 (0.1%) |
| 21 | AU | 0.53 | 0/472 | 0.57 | 0/627 |
| 21 | BU | 0.46 | 0/472 | 0.60 | 0/627 |
| 22 | CA | 0.51 | 3/69165 (0.0%) | 1.00 | 108/107896 (0.1%) |
| 23 | CB | 0.41 | 0/2828 | 0.90 | 2/4410 (0.0%) |
| 23 | DB | 0.79 | 0/2872 | 1.12 | 7/4478 (0.2%) |
| 24 | CC | 0.40 | 0/2122 | 0.76 | 2/2852 (0.1%) |
| 24 | DC | 0.57 | 0/2122 | 0.71 | 0/2852 |
| 25 | CD | 0.40 | 0/1586 | 0.71 | 0/2134 |
| 26 | CE | 0.37 | 0/1571 | 0.71 | 2/2113 (0.1%) |
| 26 | DE | 0.58 | 0/1571 | 0.66 | 0/2113 |
| 27 | CF | 0.33 | 0/1435 | 0.75 | 0/1926 |
| 27 | DF | 0.46 | 0/1435 | 0.63 | 0/1926 |
| 28 | CG | 0.39 | 0/1343 | 0.50 | 0/1816 |
| 28 | DG | 0.53 | 0/1343 | 0.61 | 0/1816 |
| 29 | CH | 0.38 | 0/1121 | 0.56 | 0/1515 |
| 29 | DH | 0.39 | 0/1121 | 0.54 | 0/1515 |
| 30 | CJ | 0.44 | 0/993 | 0.63 | 0/1341 |
| 30 | DJ | 0.48 | 0/993 | 0.66 | 0/1341 |
| 31 | CK | 0.35 | 0/1152 | 0.50 | 0/1551 |
| 31 | DK | 0.69 | 0/1152 | 0.75 | 0/1551 |
| 32 | CL | 0.39 | 0/947 | 0.73 | 0/1268 |
| 32 | DL | 0.64 | 0/955 | 0.79 | 2/1279 (0.2%) |
| 33 | CM | 0.40 | 0/1062 | 0.89 | 2/1413 (0.1%) |
| 33 | DM | 0.64 | 0/1062 | 0.71 | 0/1413 |
| 34 | CN | 0.34 | 0/1081 | 0.64 | 0/1443 |
| 34 | DN | 0.64 | 0/1092 | 0.73 | 0/1457 |
| 35 | CO | 0.40 | 0/973 | 0.74 | 1/1301 (0.1%) |
| 35 | DO | 0.69 | 0/1006 | 0.79 | 1/1345 (0.1%) |
| 36 | CP | 0.33 | 0/902 | 0.68 | 0/1209 |
| 36 | DP | 0.50 | 0/910 | 0.62 | 0/1219 |
| 37 | CQ | 0.37 | 0/929 | 0.71 | 1/1242 (0.1%) |
| 37 | DQ | 0.65 | 0/929 | 0.68 | 0/1242 |
| 38 | CR | 0.39 | 0/960 | 0.68 | 0/1278 |
| 38 | DR | 0.74 | 0/960 | 0.75 | 0/1278 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 39 | CS | 0.37 | 0/829 | 0.73 | 0/1107 |
| 39 | DS | 0.77 | 0/829 | 0.76 | 1/1107 (0.1%) |
| 40 | CT | 0.40 | 0/864 | 0.75 | 0/1156 |
| 40 | DT | 0.72 | 0/864 | 0.75 | 0/1156 |
| 41 | CU | 0.39 | 0/745 | 0.94 | 5/994 (0.5%) |
| 41 | DU | 0.59 | 0/745 | 0.72 | 0/994 |
| 42 | CV | 0.40 | 0/788 | 0.87 | 0/1051 |
| 42 | DV | 0.55 | 0/788 | 0.70 | 0/1051 |
| 43 | CW | 0.29 | 0/766 | 0.61 | 0/1025 |
| 43 | DW | 0.64 | 0/766 | 0.67 | 0/1025 |
| 44 | CX | 0.38 | 0/576 | 0.68 | 0/762 |
| 44 | DX | 0.68 | 0/598 | 0.78 | 2/790 (0.3%) |
| 45 | CY | 0.36 | 0/635 | 0.67 | 0/848 |
| 45 | DY | 0.58 | 0/635 | 0.70 | 0/848 |
| 46 | CZ | 0.34 | 0/502 | 0.77 | 0/667 |
| 46 | DZ | 0.54 | 0/502 | 0.58 | 0/667 |
| 47 | C0 | 0.34 | 0/453 | 0.69 | 0/605 |
| 47 | D0 | 0.65 | 0/467 | 0.71 | 0/623 |
| 48 | C1 | 0.42 | 0/450 | 0.73 | 0/599 |
| 48 | D1 | 0.65 | 0/450 | 0.73 | 0/599 |
| 49 | C2 | 0.43 | 0/416 | 0.71 | 0/554 |
| 49 | D2 | 0.60 | 0/421 | 0.66 | 0/561 |
| 50 | C3 | 0.46 | 0/380 | 0.81 | 0/498 |
| 50 | D3 | 0.66 | 0/380 | 0.84 | 0/498 |
| 51 | C4 | 0.37 | 0/513 | 0.70 | 0/676 |
| 51 | D4 | 0.56 | 0/513 | 0.64 | 0/676 |
| 52 | C5 | 0.38 | 0/303 | 0.98 | 1/397 (0.3%) |
| 52 | D5 | 0.62 | 0/303 | 0.81 | 0/397 |
| 53 | DA | 1.00 | 34/69295 (0.0%) | 1.31 | 473/108100 (0.4%) |
| 54 | DD | 0.72 | 0/1576 | 0.76 | 2/2119 (0.1%) |
| 55 | DI | 0.42 | 0/1037 | 0.60 | 0/1402 |
| All | All | 0.65 | 37/309204 (0.0%) | 1.02 | 752/462103 (0.2%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | BA | 0 | 1 |
| 6 | BF | 0 | 1 |
| 24 | DC | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 25 | CD | 0 | 1 |
| 30 | CJ | 0 | 1 |
| 30 | DJ | 0 | 1 |
| 32 | CL | 0 | 1 |
| 47 | C0 | 0 | 1 |
| 47 | D0 | 0 | 1 |
| 55 | DI | 0 | 1 |
| All | All | 0 | 10 |

All (37) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 22 | CA | 1936 | A | N9-C4 | -9.34 | 1.32 | 1.37 |
| 53 | DA | 463 | G | C8-N7 | 6.92 | 1.35 | 1.30 |
| 53 | DA | 1330 | C | C4-C5 | -6.51 | 1.37 | 1.43 |
| 53 | DA | 465 | G | C6-N1 | -6.50 | 1.35 | 1.39 |
| 53 | DA | 1679 | A | N7-C5 | -6.28 | 1.35 | 1.39 |
| 53 | DA | 2269 | G | C8-N7 | 6.27 | 1.34 | 1.30 |
| 53 | DA | 800 | A | C5-C4 | -6.17 | 1.34 | 1.38 |
| 53 | DA | 680 | C | N1-C6 | -5.92 | 1.33 | 1.37 |
| 53 | DA | 654 | A | N9-C4 | 5.83 | 1.41 | 1.37 |
| 53 | DA | 788 | A | N3-C4 | -5.74 | 1.31 | 1.34 |
| 53 | DA | 516 | C | P-OP2 | -5.69 | 1.39 | 1.49 |
| 53 | DA | 1607 | C | P-O5' | -5.63 | 1.54 | 1.59 |
| 53 | DA | 1847 | A | N9-C4 | 5.57 | 1.41 | 1.37 |
| 53 | DA | 573 | U | P-OP2 | -5.56 | 1.39 | 1.49 |
| 53 | DA | 2641 | G | C8-N7 | 5.55 | 1.34 | 1.30 |
| 53 | DA | 527 | C | N1-C6 | -5.49 | 1.33 | 1.37 |
| 53 | DA | 2892 | G | P-O5' | -5.43 | 1.54 | 1.59 |
| 22 | CA | 528 | A | N9-C4 | -5.35 | 1.34 | 1.37 |
| 53 | DA | 1147 | A | C6-N1 | -5.32 | 1.31 | 1.35 |
| 53 | DA | 819 | A | C6-N1 | -5.29 | 1.31 | 1.35 |
| 53 | DA | 2641 | G | N3-C4 | -5.26 | 1.31 | 1.35 |
| 53 | DA | 2040 | G | C6-N1 | -5.25 | 1.35 | 1.39 |
| 53 | DA | 2052 | A | N9-C4 | -5.25 | 1.34 | 1.37 |
| 22 | CA | 1132 | U | O3'-P | 5.24 | 1.67 | 1.61 |
| 53 | DA | 2249 | U | C2-N3 | -5.24 | 1.34 | 1.37 |
| 53 | DA | 586 | A | N3-C4 | -5.23 | 1.31 | 1.34 |
| 53 | DA | 2499 | C | P-OP1 | -5.22 | 1.40 | 1.49 |
| 53 | DA | 2336 | A | N3-C4 | -5.19 | 1.31 | 1.34 |
| 53 | DA | 30 | G | N3-C4 | -5.18 | 1.31 | 1.35 |
| 53 | DA | 1671 | U | C2-N3 | -5.16 | 1.34 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 53 | DA | 2442 | C | C4-C5 | -5.12 | 1.38 | 1.43 |
| 53 | DA | 2053 | G | O3'-P | -5.12 | 1.55 | 1.61 |
| 53 | DA | 1666 | G | N9-C4 | 5.10 | 1.42 | 1.38 |
| 53 | DA | 1263 | U | C2-N3 | -5.09 | 1.34 | 1.37 |
| 53 | DA | 1937 | A | N3-C4 | -5.08 | 1.31 | 1.34 |
| 53 | DA | 1844 | C | N1-C6 | -5.07 | 1.34 | 1.37 |
| 53 | DA | 1992 | G | N7-C5 | -5.04 | 1.36 | 1.39 |

All (752) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 53 | DA | 1997 | C | O5'-P-OP2 | -13.03 | 93.98 | 105.70 |
| 53 | DA | 574 | A | O5'-P-OP1 | -12.59 | 94.37 | 105.70 |
| 53 | DA | 914 | G | N1-C6-O6 | 12.55 | 127.43 | 119.90 |
| 22 | CA | 963 | U | O5'-P-OP2 | -12.45 | 94.50 | 105.70 |
| 22 | CA | 948 | C | O5'-P-OP1 | -11.07 | 95.74 | 105.70 |
| 53 | DA | 2499 | C | N1-C2-O2 | -10.91 | 112.35 | 118.90 |
| 53 | DA | 751 | A | O5'-P-OP1 | -10.83 | 95.95 | 105.70 |
| 53 | DA | 570 | G | C5-C6-O6 | -10.70 | 122.18 | 128.60 |
| 53 | DA | 512 | G | O4'-C1'-N9 | 10.69 | 116.75 | 108.20 |
| 1 | BA | 330 | C | O4'-C1'-N1 | 10.34 | 116.47 | 108.20 |
| 22 | CA | 2250 | G | O4'-C1'-N9 | -10.33 | 99.94 | 108.20 |
| 53 | DA | 570 | G | C4-C5-N7 | 10.17 | 114.87 | 110.80 |
| 22 | CA | 1936 | A | C2-N3-C4 | -10.09 | 105.55 | 110.60 |
| 53 | DA | 2813 | A | N1-C6-N6 | 10.06 | 124.64 | 118.60 |
| 53 | DA | 847 | U | O5'-P-OP2 | -9.90 | 96.79 | 105.70 |
| 1 | BA | 412 | A | O4'-C1'-N9 | 9.85 | 116.08 | 108.20 |
| 53 | DA | 2448 | A | O5'-P-OP2 | -9.79 | 96.89 | 105.70 |
| 5 | BE | 104 | GLY | N-CA-C | 9.67 | 137.28 | 113.10 |
| 53 | DA | 1987 | A | O5'-P-OP2 | -9.66 | 97.01 | 105.70 |
| 53 | DA | 963 | U | O5'-P-OP2 | -9.57 | 97.08 | 105.70 |
| 53 | DA | 1663 | G | O5'-P-OP2 | -9.54 | 97.12 | 105.70 |
| 1 | AA | 117 | G | O5'-P-OP2 | -9.50 | 97.15 | 105.70 |
| 1 | BA | 558 | G | O5'-P-OP1 | -9.50 | 97.15 | 105.70 |
| 53 | DA | 29 | U | O5'-P-OP2 | -9.44 | 97.21 | 105.70 |
| 53 | DA | 574 | A | O5'-P-OP2 | 9.36 | 121.94 | 110.70 |
| 53 | DA | 1648 | U | O5'-P-OP1 | -9.10 | 97.51 | 105.70 |
| 53 | DA | 2450 | A | O5'-P-OP2 | -9.06 | 97.55 | 105.70 |
| 53 | DA | 1935 | G | O5'-P-OP2 | -8.98 | 97.61 | 105.70 |
| 22 | CA | 1936 | A | N3-C4-N9 | -8.96 | 120.23 | 127.40 |
| 53 | DA | 802 | A | O5'-P-OP1 | -8.93 | 97.67 | 105.70 |
| 22 | CA | 1272 | A | O5'-P-OP1 | -8.89 | 97.70 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 53 | DA | 914 | G | C5-C6-O6 | -8.88 | 123.27 | 128.60 |
| 53 | DA | 738 | G | O5'-P-OP2 | -8.85 | 97.74 | 105.70 |
| 53 | DA | 329 | G | O5'-P-OP2 | -8.72 | 97.85 | 105.70 |
| 1 | BA | 632 | U | N3-C2-O2 | -8.67 | 116.13 | 122.20 |
| 53 | DA | 1134 | A | O5'-P-OP1 | -8.67 | 97.90 | 105.70 |
| 22 | CA | 1936 | A | N3-C4-C5 | 8.57 | 132.80 | 126.80 |
| 53 | DA | 465 | G | N3-C2-N2 | 8.57 | 125.90 | 119.90 |
| 53 | DA | 1010 | A | O5'-P-OP2 | -8.57 | 97.99 | 105.70 |
| 53 | DA | 2848 | G | O4'-C1'-N9 | 8.53 | 115.02 | 108.20 |
| 53 | DA | 1965 | C | O5'-P-OP2 | -8.45 | 98.09 | 105.70 |
| 53 | DA | 1026 | G | O5'-P-OP1 | -8.40 | 98.14 | 105.70 |
| 53 | DA | 1605 | C | N1-C2-O2 | -8.38 | 113.88 | 118.90 |
| 22 | CA | 752 | A | O4'-C1'-N9 | 8.30 | 114.84 | 108.20 |
| 22 | CA | 2250 | G | C4-N9-C1' | 8.27 | 137.25 | 126.50 |
| 53 | DA | 2275 | C | O5'-P-OP2 | -8.24 | 98.29 | 105.70 |
| 1 | BA | 209 | U | C2-N1-C1' | 8.23 | 127.58 | 117.70 |
| 53 | DA | 1272 | A | O5'-P-OP1 | -8.23 | 98.29 | 105.70 |
| 41 | CU | 3 | ARG | NE-CZ-NH1 | 8.15 | 124.38 | 120.30 |
| 1 | BA | 632 | U | N1-C2-O2 | 8.15 | 128.50 | 122.80 |
| 53 | DA | 2645 | G | O4'-C1'-N9 | 8.14 | 114.72 | 108.20 |
| 1 | BA | 1397 | C | C2-N1-C1' | 8.12 | 127.73 | 118.80 |
| 53 | DA | 1779 | U | N1-C2-O2 | -8.11 | 117.12 | 122.80 |
| 53 | DA | 974 | G | C5-C6-O6 | 8.08 | 133.45 | 128.60 |
| 1 | BA | 330 | C | C2-N1-C1' | -8.07 | 109.92 | 118.80 |
| 12 | BL | 14 | ARG | CG-CD-NE | 8.06 | 128.73 | 111.80 |
| 53 | DA | 570 | G | C6-C5-N7 | -8.05 | 125.57 | 130.40 |
| 53 | DA | 465 | G | C5-C6-O6 | 8.04 | 133.42 | 128.60 |
| 22 | CA | 2326 | C | P-O3'-C3' | 8.02 | 129.33 | 119.70 |
| 53 | DA | 914 | G | C6-C5-N7 | -8.01 | 125.59 | 130.40 |
| 53 | DA | 2868 | A | O5'-P-OP2 | -7.99 | 98.51 | 105.70 |
| 53 | DA | 463 | G | N9-C4-C5 | 7.91 | 108.56 | 105.40 |
| 53 | DA | 570 | G | N1-C6-O6 | 7.91 | 124.64 | 119.90 |
| 53 | DA | 763 | G | O5'-P-OP1 | -7.86 | 98.63 | 105.70 |
| 53 | DA | 1434 | A | O4'-C1'-N9 | 7.84 | 114.47 | 108.20 |
| 1 | BA | 1110 | A | O4'-C1'-N9 | -7.83 | 101.94 | 108.20 |
| 53 | DA | 739 | A | N1-C6-N6 | 7.78 | 123.27 | 118.60 |
| 53 | DA | 672 | C | N3-C4-C5 | 7.75 | 125.00 | 121.90 |
| 1 | BA | 452 | A | O4'-C1'-N9 | -7.75 | 102.00 | 108.20 |
| 53 | DA | 1847 | A | N7-C8-N9 | 7.74 | 117.67 | 113.80 |
| 53 | DA | 570 | G | C5-N7-C8 | -7.68 | 100.46 | 104.30 |
| 12 | BL | 85 | GLY | N-CA-C | -7.66 | 93.95 | 113.10 |
| 53 | DA | 1134 | A | OP1-P-OP2 | 7.64 | 131.06 | 119.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1 | BA | 207 | C | C6-N1-C2 | -7.63 | 117.25 | 120.30 |
| 53 | DA | 1997 | C | O5'-P-OP1 | 7.63 | 119.86 | 110.70 |
| 53 | DA | 1630 | A | O5'-P-OP2 | -7.62 | 98.84 | 105.70 |
| 22 | CA | 1171 | G | O4'-C1'-N9 | 7.62 | 114.29 | 108.20 |
| 41 | CU | 3 | ARG | N-CA-C | -7.59 | 90.52 | 111.00 |
| 1 | BA | 330 | C | C6-N1-C1' | 7.51 | 129.81 | 120.80 |
| 53 | DA | 1328 | A | O5'-P-OP2 | -7.51 | 98.94 | 105.70 |
| 1 | BA | 1042 | A | O5'-P-OP2 | -7.50 | 98.95 | 105.70 |
| 1 | BA | 1001 | C | C6-N1-C2 | -7.48 | 117.31 | 120.30 |
| 53 | DA | 704 | G | O4'-C1'-N9 | 7.48 | 114.18 | 108.20 |
| 22 | CA | 481 | G | O4'-C1'-N9 | 7.47 | 114.17 | 108.20 |
| 53 | DA | 2820 | A | C8-N9-C4 | 7.45 | 108.78 | 105.80 |
| 22 | CA | 528 | A | C2-N3-C4 | -7.45 | 106.88 | 110.60 |
| 22 | CA | 2425 | A | P-O3'-C3' | 7.42 | 128.60 | 119.70 |
| 44 | DX | 39 | ARG | NE-CZ-NH1 | 7.42 | 124.01 | 120.30 |
| 53 | DA | 12 | U | C2-N1-C1' | 7.42 | 126.60 | 117.70 |
| 53 | DA | 1584 | U | N1-C2-O2 | 7.40 | 127.98 | 122.80 |
| 53 | DA | 481 | G | O4'-C1'-N9 | 7.40 | 114.12 | 108.20 |
| 53 | DA | 807 | U | N3-C4-O4 | 7.36 | 124.55 | 119.40 |
| 53 | DA | 465 | G | N1-C2-N2 | -7.35 | 109.58 | 116.20 |
| 53 | DA | 1584 | U | C2-N1-C1' | 7.35 | 126.52 | 117.70 |
| 1 | BA | 211 | G | C4-N9-C1' | 7.34 | 136.04 | 126.50 |
| 22 | CA | 943 | A | O5'-P-OP2 | -7.34 | 99.10 | 105.70 |
| 39 | DS | 68 | ARG | NE-CZ-NH1 | -7.33 | 116.63 | 120.30 |
| 22 | CA | 995 | C | O4'-C1'-N1 | -7.33 | 102.34 | 108.20 |
| 1 | BA | 183 | C | C2-N1-C1' | 7.32 | 126.85 | 118.80 |
| 53 | DA | 1784 | A | N1-C6-N6 | 7.32 | 122.99 | 118.60 |
| 1 | BA | 467 | U | C2-N1-C1' | 7.30 | 126.47 | 117.70 |
| 53 | DA | 1271 | G | OP1-P-OP2 | -7.30 | 108.64 | 119.60 |
| 53 | DA | 116 | C | N3-C4-N4 | -7.29 | 112.90 | 118.00 |
| 53 | DA | 2813 | A | C5-C6-N6 | -7.28 | 117.88 | 123.70 |
| 22 | CA | 511 | U | O5'-P-OP2 | -7.27 | 99.16 | 105.70 |
| 33 | CM | 52 | GLY | N-CA-C | -7.25 | 94.98 | 113.10 |
| 53 | DA | 140 | C | C6-N1-C2 | -7.24 | 117.41 | 120.30 |
| 53 | DA | 2046 | G | C2-N3-C4 | -7.23 | 108.29 | 111.90 |
| 53 | DA | 731 | C | O5'-P-OP2 | -7.20 | 99.22 | 105.70 |
| 53 | DA | 2036 | C | O5'-P-OP2 | -7.19 | 99.23 | 105.70 |
| 1 | BA | 576 | C | O5'-P-OP2 | -7.18 | 99.23 | 105.70 |
| 53 | DA | 1220 | G | N1-C2-N2 | -7.18 | 109.74 | 116.20 |
| 1 | BA | 532 | A | N1-C6-N6 | 7.17 | 122.90 | 118.60 |
| 22 | CA | 2072 | C | O5'-P-OP2 | -7.17 | 99.25 | 105.70 |
| 53 | DA | 12 | U | C6-N1-C2 | -7.17 | 116.70 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 53 | DA | 2490 | G | O5'-P-OP2 | -7.15 | 99.26 | 105.70 |
| 53 | DA | 463 | G | C8-N9-C4 | -7.14 | 103.54 | 106.40 |
| 53 | DA | 946 | C | N1-C2-O2 | -7.12 | 114.63 | 118.90 |
| 53 | DA | 181 | A | N9-C4-C5 | 7.12 | 108.65 | 105.80 |
| 53 | DA | 2575 | C | N1-C2-O2 | 7.10 | 123.16 | 118.90 |
| 53 | DA | 1937 | A | O4'-C1'-N9 | 7.08 | 113.86 | 108.20 |
| 1 | BA | 632 | U | C2-N1-C1' | 7.08 | 126.19 | 117.70 |
| 53 | DA | 102 | U | C2-N1-C1' | 7.08 | 126.19 | 117.70 |
| 1 | BA | 4 | U | C2-N1-C1' | 7.06 | 126.17 | 117.70 |
| 22 | CA | 900 | A | O4'-C1'-N9 | 7.04 | 113.83 | 108.20 |
| 53 | DA | 139 | U | N1-C2-O2 | 7.03 | 127.72 | 122.80 |
| 53 | DA | 2263 | C | N3-C4-C5 | 7.02 | 124.71 | 121.90 |
| 53 | DA | 2883 | A | O5'-P-OP2 | -7.02 | 99.38 | 105.70 |
| 53 | DA | 2641 | G | C5-C6-O6 | 7.00 | 132.80 | 128.60 |
| 22 | CA | 1378 | A | P-O3'-C3' | 6.99 | 128.09 | 119.70 |
| 53 | DA | 2641 | G | N3-C4-N9 | -6.98 | 121.81 | 126.00 |
| 53 | DA | 1286 | A | O5'-P-OP2 | -6.98 | 99.42 | 105.70 |
| 53 | DA | 2407 | A | O5'-P-OP1 | -6.98 | 99.42 | 105.70 |
| 53 | DA | 1668 | A | O5'-P-OP2 | -6.97 | 99.43 | 105.70 |
| 53 | DA | 1768 | C | O5'-P-OP2 | -6.97 | 99.43 | 105.70 |
| 53 | DA | 1706 | C | O4'-C1'-N1 | 6.96 | 113.77 | 108.20 |
| 22 | CA | 2225 | A | P-O3'-C3' | 6.96 | 128.06 | 119.70 |
| 53 | DA | 208 | C | O5'-P-OP2 | -6.96 | 99.44 | 105.70 |
| 53 | DA | 672 | C | C5-C4-N4 | -6.94 | 115.34 | 120.20 |
| 1 | BA | 792 | A | O4'-C1'-N9 | 6.92 | 113.74 | 108.20 |
| 53 | DA | 570 | G | N9-C4-C5 | -6.91 | 102.64 | 105.40 |
| 53 | DA | 2820 | A | N1-C6-N6 | 6.91 | 122.74 | 118.60 |
| 22 | CA | 757 | G | N3-C4-C5 | 6.89 | 132.04 | 128.60 |
| 53 | DA | 1602 | U | N3-C4-O4 | -6.89 | 114.58 | 119.40 |
| 1 | AA | 4 | U | C2-N1-C1' | 6.88 | 125.95 | 117.70 |
| 1 | AA | 1279 | G | C4-N9-C1' | 6.87 | 135.43 | 126.50 |
| 53 | DA | 1297 | C | N3-C2-O2 | -6.87 | 117.09 | 121.90 |
| 53 | DA | 671 | C | C6-N1-C2 | -6.87 | 117.55 | 120.30 |
| 8 | BH | 68 | GLY | N-CA-C | -6.86 | 95.95 | 113.10 |
| 53 | DA | 1171 | G | C8-N9-C4 | -6.85 | 103.66 | 106.40 |
| 1 | BA | 1109 | C | P-O3'-C3' | 6.84 | 127.91 | 119.70 |
| 53 | DA | 950 | G | O5'-P-OP2 | -6.83 | 99.55 | 105.70 |
| 22 | CA | 34 | U | C5'-C4'-O4' | -6.81 | 100.93 | 109.10 |
| 53 | DA | 1155 | A | N1-C6-N6 | -6.81 | 114.51 | 118.60 |
| 20 | BT | 66 | LEU | CA-CB-CG | 6.81 | 130.95 | 115.30 |
| 53 | DA | 2056 | G | O4'-C1'-N9 | -6.78 | 102.78 | 108.20 |
| 1 | AA | 887 | G | O5'-P-OP2 | -6.78 | 99.60 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 53 | DA | 1270 | C | O5'-P-OP2 | -6.74 | 99.63 | 105.70 |
| 53 | DA | 2808 | G | O5'-P-OP2 | -6.74 | 99.64 | 105.70 |
| 53 | DA | 2681 | C | O5'-P-OP2 | -6.73 | 99.64 | 105.70 |
| 1 | AA | 330 | C | C2-N3-C4 | 6.72 | 123.26 | 119.90 |
| 53 | DA | 1162 | G | O5'-P-OP2 | -6.67 | 99.69 | 105.70 |
| 1 | BA | 573 | A | O4'-C1'-N9 | -6.67 | 102.86 | 108.20 |
| 1 | BA | 842 | U | C5-C6-N1 | 6.67 | 126.03 | 122.70 |
| 53 | DA | 101 | A | O4'-C1'-N9 | 6.66 | 113.53 | 108.20 |
| 1 | BA | 1012 | A | N3-C4-N9 | -6.66 | 122.08 | 127.40 |
| 22 | CA | 140 | C | N1-C2-O2 | 6.65 | 122.89 | 118.90 |
| 53 | DA | 2033 | A | O5'-P-OP1 | -6.65 | 99.71 | 105.70 |
| 53 | DA | 2638 | G | O4'-C1'-N9 | 6.65 | 113.52 | 108.20 |
| 53 | DA | 1819 | A | N1-C6-N6 | 6.64 | 122.58 | 118.60 |
| 53 | DA | 984 | A | O4'-C1'-N9 | 6.64 | 113.51 | 108.20 |
| 1 | BA | 1167 | A | C8-N9-C4 | -6.61 | 103.15 | 105.80 |
| 53 | DA | 830 | G | O5'-P-OP1 | -6.61 | 99.75 | 105.70 |
| 1 | BA | 573 | A | O5'-P-OP1 | -6.60 | 99.76 | 105.70 |
| 53 | DA | 2889 | C | N1-C2-O2 | -6.58 | 114.95 | 118.90 |
| 53 | DA | 2618 | G | N3-C2-N2 | -6.58 | 115.29 | 119.90 |
| 53 | DA | 2712 | C | N3-C4-C5 | 6.58 | 124.53 | 121.90 |
| 22 | CA | 2884 | U | N3-C2-O2 | -6.57 | 117.60 | 122.20 |
| 53 | DA | 26 | G | C2-N3-C4 | -6.57 | 108.61 | 111.90 |
| 53 | DA | 2815 | C | N1-C2-O2 | -6.57 | 114.96 | 118.90 |
| 22 | CA | 545 | U | N3-C2-O2 | -6.56 | 117.61 | 122.20 |
| 22 | CA | 646 | U | P-O3'-C3' | 6.54 | 127.55 | 119.70 |
| 53 | DA | 751 | A | O5'-P-OP2 | 6.54 | 118.55 | 110.70 |
| 53 | DA | 1967 | C | N3-C4-C5 | -6.54 | 119.29 | 121.90 |
| 15 | BO | 87 | LEU | CA-CB-CG | 6.53 | 130.33 | 115.30 |
| 53 | DA | 116 | C | C5-C4-N4 | 6.53 | 124.77 | 120.20 |
| 53 | DA | 2390 | U | O5'-P-OP2 | -6.53 | 99.82 | 105.70 |
| 1 | AA | 330 | C | C5-C6-N1 | 6.53 | 124.26 | 121.00 |
| 32 | DL | 70 | ARG | NE-CZ-NH2 | -6.52 | 117.04 | 120.30 |
| 53 | DA | 807 | U | C5-C4-O4 | -6.51 | 121.99 | 125.90 |
| 53 | DA | 181 | A | C8-N9-C4 | -6.50 | 103.20 | 105.80 |
| 53 | DA | 1847 | A | C8-N9-C4 | -6.49 | 103.20 | 105.80 |
| 53 | DA | 1311 | G | O4'-C1'-N9 | 6.48 | 113.39 | 108.20 |
| 22 | CA | 2250 | G | C8-N9-C1' | -6.48 | 118.58 | 127.00 |
| 53 | DA | 2249 | U | C4-C5-C6 | -6.48 | 115.81 | 119.70 |
| 53 | DA | 1788 | C | C5-C4-N4 | -6.48 | 115.67 | 120.20 |
| 6 | BF | 92 | THR | N-CA-C | 6.46 | 128.46 | 111.00 |
| 22 | CA | 2585 | U | C5'-C4'-O4' | -6.46 | 101.34 | 109.10 |
| 53 | DA | 1779 | U | N3-C2-O2 | 6.46 | 126.72 | 122.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 53 | DA | 12 | U | N3-C2-O2 | -6.46 | 117.68 | 122.20 |
| 53 | DA | 1020 | A | N1-C6-N6 | 6.45 | 122.47 | 118.60 |
| 53 | DA | 978 | G | N3-C2-N2 | 6.45 | 124.42 | 119.90 |
| 53 | DA | 1300 | G | O5'-P-OP2 | -6.44 | 99.90 | 105.70 |
| 53 | DA | 1171 | G | C4-N9-C1' | 6.44 | 134.87 | 126.50 |
| 1 | BA | 328 | C | C2-N1-C1' | 6.43 | 125.88 | 118.80 |
| 22 | CA | 2250 | G | N7-C8-N9 | 6.42 | 116.31 | 113.10 |
| 53 | DA | 1261 | C | O5'-P-OP2 | -6.42 | 99.92 | 105.70 |
| 53 | DA | 2008 | C | O5'-P-OP2 | -6.42 | 99.92 | 105.70 |
| 53 | DA | 2424 | C | N3-C4-N4 | -6.42 | 113.51 | 118.00 |
| 23 | DB | 97 | C | N1-C2-O2 | -6.40 | 115.06 | 118.90 |
| 53 | DA | 1009 | A | OP1-P-OP2 | -6.40 | 110.00 | 119.60 |
| 53 | DA | 2027 | G | N1-C6-O6 | -6.39 | 116.06 | 119.90 |
| 23 | DB | 81 | G | C5-C6-O6 | -6.39 | 124.76 | 128.60 |
| 53 | DA | 139 | U | N3-C2-O2 | -6.39 | 117.73 | 122.20 |
| 53 | DA | 1257 | C | C6-N1-C2 | 6.38 | 122.85 | 120.30 |
| 53 | DA | 202 | U | N3-C2-O2 | -6.37 | 117.74 | 122.20 |
| 53 | DA | 1313 | U | C2-N1-C1' | 6.37 | 125.34 | 117.70 |
| 53 | DA | 299 | A | O5'-P-OP2 | -6.35 | 99.98 | 105.70 |
| 1 | BA | 183 | C | N1-C2-O2 | 6.35 | 122.71 | 118.90 |
| 53 | DA | 2518 | A | OP2-P-O3' | 6.34 | 119.15 | 105.20 |
| 1 | BA | 532 | A | C5-C6-N6 | -6.33 | 118.64 | 123.70 |
| 1 | AA | 1053 | G | OP2-P-O3' | 6.32 | 119.11 | 105.20 |
| 53 | DA | 181 | A | N1-C6-N6 | -6.31 | 114.81 | 118.60 |
| 1 | BA | 328 | C | C6-N1-C2 | -6.29 | 117.78 | 120.30 |
| 53 | DA | 914 | G | C4-C5-N7 | 6.29 | 113.32 | 110.80 |
| 53 | DA | 1311 | G | N1-C6-O6 | 6.29 | 123.67 | 119.90 |
| 22 | CA | 2250 | G | C6-C5-N7 | -6.28 | 126.63 | 130.40 |
| 1 | BA | 1397 | C | N1-C2-O2 | 6.27 | 122.66 | 118.90 |
| 22 | CA | 2566 | A | O4'-C1'-N9 | 6.27 | 113.21 | 108.20 |
| 19 | BS | 10 | PHE | CB-CG-CD1 | -6.26 | 116.42 | 120.80 |
| 53 | DA | 748 | G | O4'-C1'-N9 | 6.25 | 113.20 | 108.20 |
| 53 | DA | 1190 | G | N3-C4-C5 | 6.24 | 131.72 | 128.60 |
| 53 | DA | 670 | A | O4'-C1'-N9 | -6.24 | 103.21 | 108.20 |
| 22 | CA | 1174 | U | N3-C2-O2 | -6.24 | 117.83 | 122.20 |
| 1 | AA | 579 | A | O5'-P-OP2 | -6.23 | 100.09 | 105.70 |
| 53 | DA | 1709 | U | C5-C4-O4 | -6.23 | 122.16 | 125.90 |
| 22 | CA | 1584 | U | C2-N1-C1' | 6.22 | 125.17 | 117.70 |
| 53 | DA | 1784 | A | C5-C6-N6 | -6.22 | 118.72 | 123.70 |
| 1 | BA | 78 | A | C8-N9-C4 | -6.22 | 103.31 | 105.80 |
| 53 | DA | 2614 | A | N1-C6-N6 | 6.21 | 122.33 | 118.60 |
| 22 | CA | 783 | A | N1-C6-N6 | 6.21 | 122.33 | 118.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 7 | BG | 54 | SER | N-CA-C | -6.20 | 94.25 | 111.00 |
| 53 | DA | 1330 | C | N3-C4-N4 | 6.20 | 122.34 | 118.00 |
| 22 | CA | 2585 | U | N1-C1'-C2' | -6.19 | 105.19 | 112.00 |
| 53 | DA | 997 | G | C5-C6-O6 | 6.19 | 132.31 | 128.60 |
| 53 | DA | 1297 | C | N1-C2-O2 | 6.18 | 122.61 | 118.90 |
| 53 | DA | 1709 | U | N3-C4-O4 | 6.18 | 123.73 | 119.40 |
| 1 | BA | 553 | A | O5'-P-OP2 | -6.18 | 100.14 | 105.70 |
| 22 | CA | 140 | C | P-O3'-C3' | 6.17 | 127.10 | 119.70 |
| 41 | CU | 3 | ARG | NE-CZ-NH2 | -6.17 | 117.22 | 120.30 |
| 22 | CA | 2689 | U | O4'-C1'-N1 | -6.16 | 103.28 | 108.20 |
| 23 | CB | 15 | A | P-O3'-C3' | 6.16 | 127.09 | 119.70 |
| 53 | DA | 1828 | G | O5'-P-OP2 | -6.16 | 100.16 | 105.70 |
| 53 | DA | 1208 | C | N3-C2-O2 | -6.15 | 117.59 | 121.90 |
| 22 | CA | 528 | A | C5-C6-N1 | -6.15 | 114.63 | 117.70 |
| 53 | DA | 2820 | A | C2-N3-C4 | -6.14 | 107.53 | 110.60 |
| 53 | DA | 2715 | C | C6-N1-C2 | -6.13 | 117.85 | 120.30 |
| 53 | DA | 17 | G | N3-C4-C5 | 6.12 | 131.66 | 128.60 |
| 52 | C5 | 12 | ARG | CG-CD-NE | -6.12 | 98.95 | 111.80 |
| 22 | CA | 1943 | U | C2-N3-C4 | 6.11 | 130.67 | 127.00 |
| 1 | AA | 330 | C | C6-N1-C2 | -6.11 | 117.86 | 120.30 |
| 53 | DA | 2050 | C | N3-C4-C5 | 6.11 | 124.34 | 121.90 |
| 53 | DA | 528 | A | O5'-P-OP1 | 6.10 | 118.02 | 110.70 |
| 22 | CA | 2430 | A | O4'-C1'-N9 | 6.10 | 113.08 | 108.20 |
| 53 | DA | 334 | C | C6-N1-C2 | 6.09 | 122.74 | 120.30 |
| 53 | DA | 2448 | A | O5'-P-OP1 | -6.09 | 100.22 | 105.70 |
| 1 | AA | 971 | G | O4'-C1'-N9 | 6.09 | 113.07 | 108.20 |
| 53 | DA | 2301 | C | C6-N1-C2 | -6.08 | 117.87 | 120.30 |
| 53 | DA | 370 | G | O5'-P-OP2 | -6.08 | 100.23 | 105.70 |
| 53 | DA | 1116 | G | N1-C6-O6 | -6.06 | 116.26 | 119.90 |
| 53 | DA | 687 | C | O5'-P-OP2 | -6.06 | 100.25 | 105.70 |
| 1 | AA | 321 | A | O5'-P-OP2 | -6.05 | 100.25 | 105.70 |
| 53 | DA | 752 | A | N9-C4-C5 | 6.05 | 108.22 | 105.80 |
| 22 | CA | 793 | A | O5'-P-OP2 | -6.04 | 100.26 | 105.70 |
| 53 | DA | 1985 | C | O5'-P-OP2 | -6.04 | 100.26 | 105.70 |
| 53 | DA | 194 | G | N3-C4-C5 | 6.03 | 131.62 | 128.60 |
| 53 | DA | 2835 | A | O4'-C1'-N9 | -6.03 | 103.37 | 108.20 |
| 22 | CA | 1607 | C | O4'-C1'-N1 | -6.03 | 103.38 | 108.20 |
| 53 | DA | 140 | C | N3-C2-O2 | -6.03 | 117.68 | 121.90 |
| 53 | DA | 2813 | A | C5-N7-C8 | -6.03 | 100.89 | 103.90 |
| 1 | AA | 328 | C | N1-C2-O2 | 6.03 | 122.52 | 118.90 |
| 53 | DA | 1153 | C | N1-C2-O2 | 6.03 | 122.52 | 118.90 |
| 1 | AA | 844 | G | C2-N3-C4 | 6.01 | 114.91 | 111.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 53 | DA | 2028 | U | C5-C4-O4 | -6.00 | 122.30 | 125.90 |
| 1 | AA | 330 | C | C2-N1-C1' | 6.00 | 125.40 | 118.80 |
| 53 | DA | 328 | U | OP1-P-O3' | 6.00 | 118.41 | 105.20 |
| 1 | BA | 211 | G | C8-N9-C1' | -6.00 | 119.20 | 127.00 |
| 53 | DA | 2006 | C | N1-C2-O2 | 6.00 | 122.50 | 118.90 |
| 22 | CA | 1914 | C | N1-C2-O2 | 5.99 | 122.50 | 118.90 |
| 53 | DA | 1666 | G | N1-C6-O6 | -5.99 | 116.31 | 119.90 |
| 53 | DA | 1116 | G | C5-C6-O6 | 5.98 | 132.19 | 128.60 |
| 53 | DA | 246 | C | O5'-P-OP2 | -5.98 | 100.32 | 105.70 |
| 22 | CA | 2308 | G | O4'-C1'-N9 | 5.98 | 112.98 | 108.20 |
| 53 | DA | 2824 | C | C6-N1-C2 | -5.97 | 117.91 | 120.30 |
| 22 | CA | 1584 | U | N3-C2-O2 | -5.97 | 118.02 | 122.20 |
| 22 | CA | 1828 | G | O5'-P-OP2 | -5.97 | 100.33 | 105.70 |
| 35 | DO | 2 | ARG | NE-CZ-NH2 | -5.97 | 117.32 | 120.30 |
| 1 | BA | 576 | C | O5'-P-OP1 | 5.96 | 117.85 | 110.70 |
| 53 | DA | 2641 | G | N1-C6-O6 | -5.96 | 116.32 | 119.90 |
| 1 | BA | 1003 | G | C4-N9-C1' | 5.95 | 134.24 | 126.50 |
| 53 | DA | 465 | G | N1-C6-O6 | -5.95 | 116.33 | 119.90 |
| 22 | CA | 783 | A | N7-C8-N9 | 5.95 | 116.78 | 113.80 |
| 22 | CA | 12 | U | N3-C2-O2 | -5.95 | 118.03 | 122.20 |
| 22 | CA | 793 | A | C8-N9-C4 | 5.95 | 108.18 | 105.80 |
| 22 | CA | 1807 | G | O4'-C1'-N9 | 5.94 | 112.95 | 108.20 |
| 22 | CA | 135 | U | C2-N1-C1' | 5.94 | 124.83 | 117.70 |
| 53 | DA | 1223 | G | C8-N9-C4 | 5.94 | 108.78 | 106.40 |
| 53 | DA | 2820 | A | OP1-P-O3' | 5.92 | 118.23 | 105.20 |
| 1 | AA | 872 | A | O4'-C1'-N9 | 5.92 | 112.94 | 108.20 |
| 22 | CA | 635 | C | C6-N1-C2 | -5.92 | 117.93 | 120.30 |
| 53 | DA | 2821 | A | N9-C4-C5 | -5.92 | 103.43 | 105.80 |
| 22 | CA | 783 | A | C8-N9-C4 | -5.91 | 103.44 | 105.80 |
| 53 | DA | 744 | U | N3-C4-O4 | 5.91 | 123.53 | 119.40 |
| 53 | DA | 1630 | A | N1-C6-N6 | -5.90 | 115.06 | 118.60 |
| 1 | BA | 496 | A | O4'-C1'-N9 | 5.90 | 112.92 | 108.20 |
| 22 | CA | 1584 | U | N1-C2-O2 | 5.89 | 126.93 | 122.80 |
| 53 | DA | 1236 | G | O4'-C1'-N9 | 5.89 | 112.91 | 108.20 |
| 1 | BA | 573 | A | P-O3'-C3' | 5.89 | 126.76 | 119.70 |
| 1 | BA | 1054 | C | C6-N1-C2 | -5.88 | 117.95 | 120.30 |
| 53 | DA | 1339 | G | C5-C6-O6 | -5.88 | 125.07 | 128.60 |
| 1 | BA | 27 | G | N1-C6-O6 | 5.88 | 123.42 | 119.90 |
| 22 | CA | 38 | A | O5'-P-OP2 | -5.87 | 100.42 | 105.70 |
| 22 | CA | 528 | A | O4'-C1'-N9 | -5.86 | 103.51 | 108.20 |
| 53 | DA | 1429 | G | C5-C6-O6 | 5.86 | 132.12 | 128.60 |
| 22 | CA | 2585 | U | O4'-C1'-N1 | -5.86 | 103.51 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 53 | DA | 1238 | G | O5'-P-OP2 | -5.86 | 100.43 | 105.70 |
| 53 | DA | 923 | G | N1-C6-O6 | -5.85 | 116.39 | 119.90 |
| 53 | DA | 2629 | U | O5'-P-OP2 | -5.85 | 100.44 | 105.70 |
| 1 | AA | 328 | C | N3-C2-O2 | -5.84 | 117.81 | 121.90 |
| 53 | DA | 1190 | G | C2-N3-C4 | -5.84 | 108.98 | 111.90 |
| 22 | CA | 1943 | U | C5-C4-O4 | 5.84 | 129.40 | 125.90 |
| 1 | BA | 1397 | C | C6-N1-C2 | -5.83 | 117.97 | 120.30 |
| 53 | DA | 140 | C | N1-C2-O2 | 5.83 | 122.40 | 118.90 |
| 53 | DA | 999 | U | C5-C4-O4 | 5.83 | 129.40 | 125.90 |
| 53 | DA | 2027 | G | C5-C6-N1 | 5.83 | 114.41 | 111.50 |
| 53 | DA | 592 | A | C6-N1-C2 | -5.82 | 115.11 | 118.60 |
| 24 | CC | 213 | TRP | CA-CB-CG | 5.82 | 124.76 | 113.70 |
| 22 | CA | 140 | C | N3-C2-O2 | -5.82 | 117.83 | 121.90 |
| 1 | BA | 183 | C | C6-N1-C1' | -5.82 | 113.82 | 120.80 |
| 53 | DA | 484 | C | N1-C2-O2 | 5.81 | 122.39 | 118.90 |
| 53 | DA | 1394 | U | O4'-C1'-N1 | -5.81 | 103.55 | 108.20 |
| 53 | DA | 1425 | G | C8-N9-C4 | -5.81 | 104.08 | 106.40 |
| 53 | DA | 102 | U | N3-C2-O2 | -5.81 | 118.14 | 122.20 |
| 53 | DA | 521 | U | C6-N1-C2 | -5.80 | 117.52 | 121.00 |
| 53 | DA | 1133 | A | O4'-C1'-N9 | 5.80 | 112.84 | 108.20 |
| 18 | BR | 55 | LEU | CA-CB-CG | 5.79 | 128.63 | 115.30 |
| 53 | DA | 784 | G | OP1-P-O3' | 5.79 | 117.95 | 105.20 |
| 53 | DA | 1584 | U | C6-N1-C1' | -5.79 | 113.09 | 121.20 |
| 53 | DA | 2282 | G | O4'-C1'-N9 | 5.79 | 112.83 | 108.20 |
| 1 | BA | 209 | U | N1-C2-O2 | 5.79 | 126.85 | 122.80 |
| 53 | DA | 1187 | G | N1-C6-O6 | -5.79 | 116.43 | 119.90 |
| 1 | BA | 485 | U | C2-N1-C1' | 5.79 | 124.64 | 117.70 |
| 1 | BA | 530 | G | C4-N9-C1' | 5.79 | 134.02 | 126.50 |
| 22 | CA | 545 | U | C2-N1-C1' | 5.77 | 124.63 | 117.70 |
| 53 | DA | 1679 | A | O5'-P-OP2 | -5.77 | 100.51 | 105.70 |
| 53 | DA | 1984 | G | O5'-P-OP2 | -5.76 | 100.52 | 105.70 |
| 1 | BA | 468 | A | N7-C8-N9 | 5.75 | 116.68 | 113.80 |
| 53 | DA | 212 | G | N9-C4-C5 | 5.75 | 107.70 | 105.40 |
| 53 | DA | 2813 | A | C4-C5-N7 | 5.75 | 113.58 | 110.70 |
| 1 | BA | 1001 | C | C5-C6-N1 | 5.75 | 123.88 | 121.00 |
| 1 | AA | 1279 | G | N7-C8-N9 | 5.74 | 115.97 | 113.10 |
| 1 | AA | 330 | C | N1-C2-O2 | 5.74 | 122.34 | 118.90 |
| 53 | DA | 655 | A | N1-C6-N6 | -5.74 | 115.16 | 118.60 |
| 53 | DA | 1329 | U | N3-C4-O4 | 5.74 | 123.42 | 119.40 |
| 53 | DA | 1780 | A | OP1-P-OP2 | -5.74 | 111.00 | 119.60 |
| 53 | DA | 914 | G | OP2-P-O3' | 5.73 | 117.81 | 105.20 |
| 6 | BF | 35 | LYS | CA-CB-CG | 5.73 | 126.00 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | CA | 2585 | U | N3-C2-O2 | -5.72 | 118.19 | 122.20 |
| 53 | DA | 13 | A | OP1-P-O3' | 5.72 | 117.79 | 105.20 |
| 22 | CA | 12 | U | C6-N1-C2 | -5.72 | 117.57 | 121.00 |
| 53 | DA | 181 | A | C5-C6-N6 | 5.71 | 128.27 | 123.70 |
| 53 | DA | 446 | G | N1-C6-O6 | 5.71 | 123.33 | 119.90 |
| 53 | DA | 8 | C | N1-C2-O2 | -5.71 | 115.47 | 118.90 |
| 1 | BA | 1012 | A | C8-N9-C4 | -5.71 | 103.52 | 105.80 |
| 22 | CA | 818 | G | P-O3'-C3' | 5.71 | 126.55 | 119.70 |
| 53 | DA | 395 | U | O4'-C1'-N1 | 5.71 | 112.76 | 108.20 |
| 22 | CA | 1368 | G | C8-N9-C4 | -5.70 | 104.12 | 106.40 |
| 53 | DA | 205 | G | O4'-C1'-N9 | 5.70 | 112.76 | 108.20 |
| 53 | DA | 1671 | U | N3-C4-O4 | -5.70 | 115.41 | 119.40 |
| 53 | DA | 1220 | G | C2-N3-C4 | -5.70 | 109.05 | 111.90 |
| 1 | AA | 412 | A | N9-C1'-C2' | 5.69 | 121.40 | 114.00 |
| 22 | CA | 2250 | G | C8-N9-C4 | -5.69 | 104.12 | 106.40 |
| 53 | DA | 1965 | C | O5'-P-OP1 | 5.69 | 117.53 | 110.70 |
| 53 | DA | 547 | A | C8-N9-C4 | -5.69 | 103.53 | 105.80 |
| 22 | CA | 613 | A | O4'-C1'-N9 | -5.69 | 103.65 | 108.20 |
| 53 | DA | 2465 | C | O5'-P-OP2 | -5.68 | 100.58 | 105.70 |
| 53 | DA | 1182 | G | N3-C4-C5 | -5.68 | 125.76 | 128.60 |
| 22 | CA | 1265 | A | O5'-P-OP2 | -5.68 | 100.59 | 105.70 |
| 53 | DA | 914 | G | C5-N7-C8 | -5.68 | 101.46 | 104.30 |
| 53 | DA | 2258 | C | N1-C2-O2 | 5.68 | 122.31 | 118.90 |
| 22 | CA | 1174 | U | N1-C2-O2 | 5.67 | 126.77 | 122.80 |
| 24 | CC | 196 | GLY | N-CA-C | 5.67 | 127.29 | 113.10 |
| 22 | CA | 764 | A | N1-C6-N6 | -5.67 | 115.20 | 118.60 |
| 23 | DB | 81 | G | C4-C5-N7 | 5.67 | 113.07 | 110.80 |
| 37 | CQ | 114 | LEU | CA-CB-CG | 5.67 | 128.34 | 115.30 |
| 53 | DA | 13 | A | C6-N1-C2 | -5.67 | 115.20 | 118.60 |
| 53 | DA | 102 | U | N1-C2-O2 | 5.67 | 126.77 | 122.80 |
| 53 | DA | 2336 | A | C6-N1-C2 | -5.67 | 115.20 | 118.60 |
| 53 | DA | 1936 | A | C8-N9-C4 | 5.66 | 108.07 | 105.80 |
| 53 | DA | 2027 | G | C2-N3-C4 | 5.66 | 114.73 | 111.90 |
| 53 | DA | 1171 | G | N3-C4-C5 | -5.66 | 125.77 | 128.60 |
| 53 | DA | 1221 | C | N3-C4-C5 | 5.66 | 124.16 | 121.90 |
| 22 | CA | 2848 | G | N1-C6-O6 | -5.65 | 116.51 | 119.90 |
| 53 | DA | 2815 | C | N3-C2-O2 | 5.65 | 125.86 | 121.90 |
| 53 | DA | 511 | U | O5'-P-OP2 | -5.64 | 100.62 | 105.70 |
| 53 | DA | 2211 | A | N1-C6-N6 | 5.64 | 121.98 | 118.60 |
| 53 | DA | 775 | G | O4'-C1'-N9 | 5.64 | 112.71 | 108.20 |
| 1 | AA | 1279 | G | C8-N9-C1' | -5.63 | 119.68 | 127.00 |
| 22 | CA | 802 | A | O5'-P-OP1 | -5.63 | 100.64 | 105.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 1 | BA | 1531 | A | N1-C6-N6 | 5.62 | 121.97 | 118.60 |
| 1 | AA | 85 | U | C2-N1-C1' | 5.61 | 124.43 | 117.70 |
| 53 | DA | 923 | G | C5-C6-O6 | 5.61 | 131.97 | 128.60 |
| 53 | DA | 975 | A | N1-C6-N6 | -5.61 | 115.23 | 118.60 |
| 53 | DA | 997 | G | N3-C4-N9 | -5.60 | 122.64 | 126.00 |
| 22 | CA | 2723 | C | C6-N1-C2 | -5.60 | 118.06 | 120.30 |
| 53 | DA | 851 | C | O5'-P-OP2 | -5.60 | 100.66 | 105.70 |
| 53 | DA | 1649 | G | O5'-P-OP1 | -5.59 | 100.67 | 105.70 |
| 1 | BA | 209 | U | C6-N1-C1' | -5.59 | 113.37 | 121.20 |
| 53 | DA | 2072 | C | N1-C2-O2 | 5.59 | 122.25 | 118.90 |
| 1 | BA | 1110 | A | O5'-C5'-C4' | 5.58 | 122.31 | 111.70 |
| 53 | DA | 463 | G | N3-C4-N9 | -5.58 | 122.65 | 126.00 |
| 53 | DA | 789 | A | C6-N1-C2 | -5.58 | 115.25 | 118.60 |
| 5 | BE | 123 | VAL | CB-CA-C | -5.58 | 100.80 | 111.40 |
| 53 | DA | 2825 | G | C4-N9-C1' | 5.58 | 133.75 | 126.50 |
| 53 | DA | 2439 | A | N1-C6-N6 | 5.57 | 121.94 | 118.60 |
| 53 | DA | 491 | G | N9-C4-C5 | 5.56 | 107.63 | 105.40 |
| 53 | DA | 461 | C | C6-N1-C2 | -5.56 | 118.08 | 120.30 |
| 53 | DA | 1573 | G | C2-N3-C4 | -5.56 | 109.12 | 111.90 |
| 53 | DA | 2405 | G | O4'-C1'-N9 | 5.56 | 112.65 | 108.20 |
| 1 | BA | 441 | A | O5'-P-OP2 | 5.56 | 117.37 | 110.70 |
| 53 | DA | 1936 | A | N9-C4-C5 | -5.55 | 103.58 | 105.80 |
| 22 | CA | 2680 | U | P-O3'-C3' | 5.55 | 126.36 | 119.70 |
| 26 | CE | 40 | ARG | CG-CD-NE | 5.55 | 123.45 | 111.80 |
| 53 | DA | 2508 | G | O5'-P-OP2 | -5.55 | 100.71 | 105.70 |
| 53 | DA | 2834 | G | N1-C6-O6 | -5.55 | 116.57 | 119.90 |
| 1 | BA | 573 | A | OP2-P-O3' | 5.55 | 117.41 | 105.20 |
| 53 | DA | 2888[A] | C | C6-N1-C2 | -5.54 | 118.08 | 120.30 |
| 53 | DA | 2888[B] | C | C6-N1-C2 | -5.54 | 118.08 | 120.30 |
| 53 | DA | 2250 | G | C8-N9-C4 | -5.54 | 104.18 | 106.40 |
| 53 | DA | 974 | G | N1-C6-O6 | -5.54 | 116.58 | 119.90 |
| 22 | CA | 1352 | U | O4'-C1'-N1 | 5.53 | 112.63 | 108.20 |
| 53 | DA | 1958 | C | N3-C4-N4 | 5.53 | 121.87 | 118.00 |
| 53 | DA | 1153 | C | N3-C2-O2 | -5.53 | 118.03 | 121.90 |
| 53 | DA | 2799 | A | C5-C6-N6 | -5.52 | 119.28 | 123.70 |
| 53 | DA | 2807 | U | O5'-P-OP2 | -5.52 | 100.73 | 105.70 |
| 53 | DA | 837 | C | N3-C4-C5 | 5.52 | 124.11 | 121.90 |
| 53 | DA | 1730 | C | C6-N1-C2 | -5.52 | 118.09 | 120.30 |
| 44 | DX | 39 | ARG | NE-CZ-NH2 | -5.52 | 117.54 | 120.30 |
| 53 | DA | 1730 | C | N3-C2-O2 | -5.51 | 118.04 | 121.90 |
| 53 | DA | 494 | G | N3-C4-C5 | 5.51 | 131.36 | 128.60 |
| 53 | DA | 800 | A | O4'-C1'-N9 | -5.51 | 103.79 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 53 | DA | 2615 | U | O5'-P-OP1 | -5.51 | 100.74 | 105.70 |
| 33 | CM | 114 | GLY | N-CA-C | 5.51 | 126.88 | 113.10 |
| 53 | DA | 786 | C | N3-C4-C5 | 5.50 | 124.10 | 121.90 |
| 53 | DA | 526 | A | OP2-P-O3' | 5.50 | 117.29 | 105.20 |
| 1 | BA | 1110 | A | C4-N9-C1' | 5.50 | 136.19 | 126.30 |
| 53 | DA | 2386 | A | N9-C4-C5 | 5.49 | 108.00 | 105.80 |
| 53 | DA | 2297 | A | O5'-P-OP1 | -5.49 | 100.76 | 105.70 |
| 53 | DA | 1370 | C | O5'-P-OP2 | -5.49 | 100.76 | 105.70 |
| 32 | DL | 58 | LEU | CA-CB-CG | 5.49 | 127.92 | 115.30 |
| 1 | BA | 1032 | G | C4-N9-C1' | 5.49 | 133.63 | 126.50 |
| 53 | DA | 1022 | G | C4-C5-N7 | -5.49 | 108.61 | 110.80 |
| 53 | DA | 2038 | G | O5'-P-OP2 | -5.49 | 100.76 | 105.70 |
| 53 | DA | 1171 | G | N7-C8-N9 | 5.48 | 115.84 | 113.10 |
| 53 | DA | 1371 | G | C8-N9-C4 | 5.48 | 108.59 | 106.40 |
| 53 | DA | 1626 | A | C8-N9-C4 | -5.48 | 103.61 | 105.80 |
| 53 | DA | 2448 | A | OP1-P-OP2 | 5.47 | 127.81 | 119.60 |
| 23 | DB | 81 | G | C6-C5-N7 | -5.47 | 127.11 | 130.40 |
| 53 | DA | 1291 | C | O5'-P-OP2 | -5.47 | 100.78 | 105.70 |
| 53 | DA | 1958 | C | C5-C4-N4 | -5.47 | 116.37 | 120.20 |
| 1 | BA | 399 | G | C8-N9-C4 | -5.47 | 104.21 | 106.40 |
| 53 | DA | 836 | G | OP2-P-O3' | 5.47 | 117.23 | 105.20 |
| 53 | DA | 2426 | A | N9-C4-C5 | -5.47 | 103.61 | 105.80 |
| 53 | DA | 978 | G | C4-C5-N7 | 5.46 | 112.98 | 110.80 |
| 53 | DA | 545 | U | C5-C6-N1 | 5.46 | 125.43 | 122.70 |
| 53 | DA | 2683 | C | N1-C2-O2 | -5.46 | 115.62 | 118.90 |
| 53 | DA | 2807 | U | OP1-P-OP2 | 5.46 | 127.79 | 119.60 |
| 1 | AA | 183 | C | C6-N1-C2 | -5.46 | 118.12 | 120.30 |
| 22 | CA | 757 | G | N3-C4-N9 | -5.46 | 122.72 | 126.00 |
| 53 | DA | 16 | C | O5'-P-OP2 | -5.46 | 100.79 | 105.70 |
| 53 | DA | 1160 | G | N3-C4-N9 | -5.46 | 122.72 | 126.00 |
| 22 | CA | 1648 | U | O5'-P-OP1 | -5.46 | 100.79 | 105.70 |
| 53 | DA | 1671 | U | N3-C2-O2 | -5.46 | 118.38 | 122.20 |
| 22 | CA | 2884 | U | N1-C2-O2 | 5.45 | 126.62 | 122.80 |
| 22 | CA | 1937 | A | O4'-C1'-N9 | 5.45 | 112.56 | 108.20 |
| 22 | CA | 2714 | G | O5'-P-OP2 | -5.45 | 100.79 | 105.70 |
| 53 | DA | 1150 | C | C6-N1-C2 | 5.45 | 122.48 | 120.30 |
| 53 | DA | 2070 | A | N1-C6-N6 | -5.45 | 115.33 | 118.60 |
| 53 | DA | 994 | C | N3-C4-N4 | -5.45 | 114.19 | 118.00 |
| 53 | DA | 1182 | G | C8-N9-C4 | -5.45 | 104.22 | 106.40 |
| 23 | CB | 90 | C | C6-N1-C2 | -5.45 | 118.12 | 120.30 |
| 53 | DA | 2585 | U | OP1-P-O3' | 5.43 | 117.16 | 105.20 |
| 53 | DA | 2501 | C | C5-C6-N1 | 5.43 | 123.72 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 54 | DD | 77 | ARG | NE-CZ-NH1 | -5.43 | 117.58 | 120.30 |
| 53 | DA | 2281 | A | N1-C6-N6 | 5.43 | 121.86 | 118.60 |
| 22 | CA | 370 | G | O5'-P-OP2 | -5.42 | 100.82 | 105.70 |
| 53 | DA | 2844 | G | C2-N3-C4 | -5.42 | 109.19 | 111.90 |
| 1 | BA | 1397 | C | C6-N1-C1' | -5.42 | 114.30 | 120.80 |
| 53 | DA | 1147 | A | N1-C6-N6 | -5.41 | 115.35 | 118.60 |
| 53 | DA | 1602 | U | N1-C2-O2 | 5.41 | 126.59 | 122.80 |
| 53 | DA | 2715 | C | O5'-P-OP2 | -5.41 | 100.83 | 105.70 |
| 53 | DA | 2767 | C | C6-N1-C2 | -5.40 | 118.14 | 120.30 |
| 1 | AA | 1418 | A | C8-N9-C4 | -5.40 | 103.64 | 105.80 |
| 53 | DA | 1971 | U | O5'-P-OP1 | 5.40 | 117.18 | 110.70 |
| 1 | BA | 205 | A | C8-N9-C4 | -5.40 | 103.64 | 105.80 |
| 1 | BA | 922 | G | C8-N9-C4 | -5.40 | 104.24 | 106.40 |
| 1 | AA | 412 | A | O4'-C1'-N9 | 5.40 | 112.52 | 108.20 |
| 1 | AA | 22 | G | O5'-P-OP2 | -5.39 | 100.85 | 105.70 |
| 1 | BA | 1183 | U | C5'-C4'-C3' | -5.39 | 107.37 | 116.00 |
| 53 | DA | 1602 | U | C5-C4-O4 | 5.39 | 129.13 | 125.90 |
| 53 | DA | 2790 | U | O5'-P-OP2 | -5.39 | 100.85 | 105.70 |
| 53 | DA | 1022 | G | C5-C6-O6 | 5.39 | 131.83 | 128.60 |
| 53 | DA | 759 | G | C4-C5-N7 | 5.39 | 112.95 | 110.80 |
| 53 | DA | 1778 | U | OP1-P-OP2 | 5.39 | 127.68 | 119.60 |
| 22 | CA | 545 | U | P-O3'-C3' | 5.38 | 126.16 | 119.70 |
| 53 | DA | 212 | G | C8-N9-C4 | -5.38 | 104.25 | 106.40 |
| 53 | DA | 1324 | G | O4'-C1'-N9 | 5.38 | 112.51 | 108.20 |
| 53 | DA | 1659 | G | N3-C4-N9 | -5.38 | 122.77 | 126.00 |
| 53 | DA | 2799 | A | N1-C6-N6 | 5.38 | 121.83 | 118.60 |
| 53 | DA | 810 | U | N1-C2-O2 | 5.38 | 126.56 | 122.80 |
| 53 | DA | 324 | A | O5'-P-OP2 | -5.37 | 100.86 | 105.70 |
| 53 | DA | 670 | A | O5'-P-OP2 | -5.37 | 100.86 | 105.70 |
| 53 | DA | 744 | U | C5-C6-N1 | 5.37 | 125.39 | 122.70 |
| 53 | DA | 2599 | G | C4-C5-N7 | 5.37 | 112.95 | 110.80 |
| 53 | DA | 1973 | G | O5'-P-OP2 | -5.37 | 100.87 | 105.70 |
| 1 | AA | 71 | A | N1-C6-N6 | 5.37 | 121.82 | 118.60 |
| 53 | DA | 788 | A | C8-N9-C4 | -5.37 | 103.65 | 105.80 |
| 1 | BA | 1279 | G | C4-N9-C1' | 5.36 | 133.47 | 126.50 |
| 53 | DA | 1508 | A | C5-N7-C8 | -5.36 | 101.22 | 103.90 |
| 53 | DA | 1782 | U | O5'-P-OP1 | -5.36 | 100.88 | 105.70 |
| 53 | DA | 43 | G | N3-C2-N2 | -5.36 | 116.15 | 119.90 |
| 53 | DA | 1329 | U | N1-C2-O2 | -5.35 | 119.05 | 122.80 |
| 22 | CA | 135 | U | O4'-C1'-N1 | -5.35 | 103.92 | 108.20 |
| 22 | CA | 545 | U | N1-C2-O2 | 5.35 | 126.54 | 122.80 |
| 53 | DA | 1679 | A | C4-C5-C6 | 5.34 | 119.67 | 117.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 53 | DA | 2780 | G | C2-N3-C4 | -5.34 | 109.23 | 111.90 |
| 22 | CA | 2395 | C | C6-N1-C2 | -5.34 | 118.16 | 120.30 |
| 53 | DA | 663 | G | N1-C2-N2 | 5.34 | 121.00 | 116.20 |
| 53 | DA | 2250 | G | N7-C8-N9 | 5.33 | 115.77 | 113.10 |
| 53 | DA | 523 | C | O5'-P-OP2 | -5.33 | 100.90 | 105.70 |
| 53 | DA | 1584 | U | N3-C2-O2 | -5.33 | 118.47 | 122.20 |
| 53 | DA | 1016 | G | C5-C6-O6 | 5.33 | 131.80 | 128.60 |
| 22 | CA | 1914 | C | N3-C2-O2 | -5.33 | 118.17 | 121.90 |
| 53 | DA | 2789 | C | OP2-P-O3' | 5.33 | 116.92 | 105.20 |
| 53 | DA | 735 | A | C5-C6-N6 | -5.32 | 119.44 | 123.70 |
| 53 | DA | 537 | G | C4-C5-N7 | 5.32 | 112.93 | 110.80 |
| 53 | DA | 806 | C | N3-C2-O2 | -5.32 | 118.18 | 121.90 |
| 53 | DA | 2839 | G | O5'-P-OP2 | -5.32 | 100.91 | 105.70 |
| 53 | DA | 1315 | C | N1-C2-O2 | 5.32 | 122.09 | 118.90 |
| 22 | CA | 961 | C | O4'-C1'-N1 | -5.31 | 103.95 | 108.20 |
| 53 | DA | 304 | U | O5'-P-OP2 | -5.31 | 100.92 | 105.70 |
| 53 | DA | 2614 | A | C5-C6-N6 | -5.31 | 119.45 | 123.70 |
| 22 | CA | 1606 | C | O4'-C1'-N1 | 5.31 | 112.45 | 108.20 |
| 53 | DA | 2710 | C | C5-C4-N4 | 5.31 | 123.92 | 120.20 |
| 53 | DA | 24 | G | O5'-P-OP2 | -5.31 | 100.92 | 105.70 |
| 53 | DA | 68 | G | C5-C6-O6 | -5.31 | 125.42 | 128.60 |
| 53 | DA | 1329 | U | C5-C4-O4 | -5.31 | 122.72 | 125.90 |
| 53 | DA | 2430[A] | A | O5'-P-OP2 | -5.29 | 100.93 | 105.70 |
| 53 | DA | 2430[B] | A | O5'-P-OP2 | -5.29 | 100.93 | 105.70 |
| 8 | BH | 67 | GLN | N-CA-C | -5.29 | 96.71 | 111.00 |
| 53 | DA | 2820 | A | N9-C4-C5 | -5.29 | 103.68 | 105.80 |
| 53 | DA | 815 | C | O5'-P-OP2 | -5.29 | 100.94 | 105.70 |
| 22 | CA | 995 | C | C2-N1-C1' | 5.29 | 124.62 | 118.80 |
| 1 | BA | 844 | G | O4'-C1'-N9 | -5.29 | 103.97 | 108.20 |
| 22 | CA | 1936 | A | N1-C2-N3 | 5.29 | 131.94 | 129.30 |
| 53 | DA | 2046 | G | N1-C2-N2 | -5.29 | 111.44 | 116.20 |
| 1 | BA | 210 | C | C6-N1-C2 | -5.29 | 118.19 | 120.30 |
| 22 | CA | 1272 | A | O4'-C1'-N9 | -5.28 | 103.97 | 108.20 |
| 53 | DA | 1330 | C | C5-C4-N4 | -5.28 | 116.50 | 120.20 |
| 1 | BA | 209 | U | N3-C2-O2 | -5.28 | 118.50 | 122.20 |
| 53 | DA | 885 | C | C6-N1-C2 | -5.28 | 118.19 | 120.30 |
| 53 | DA | 2264 | C | N3-C4-N4 | -5.28 | 114.30 | 118.00 |
| 1 | BA | 1012 | A | O4'-C1'-N9 | 5.28 | 112.42 | 108.20 |
| 53 | DA | 1602 | U | O4'-C1'-N1 | 5.28 | 112.42 | 108.20 |
| 53 | DA | 2825 | G | N3-C4-C5 | -5.28 | 125.96 | 128.60 |
| 53 | DA | 2366 | A | O5'-P-OP2 | -5.27 | 100.95 | 105.70 |
| 53 | DA | 2820 | A | N3-C4-C5 | 5.27 | 130.49 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 53 | DA | 570 | G | OP2-P-O3' | 5.27 | 116.79 | 105.20 |
| 53 | DA | 949 | G | OP1-P-OP2 | 5.27 | 127.50 | 119.60 |
| 1 | BA | 1364 | U | C2-N1-C1' | 5.26 | 124.01 | 117.70 |
| 1 | BA | 266 | G | O4'-C1'-N9 | -5.26 | 103.99 | 108.20 |
| 1 | BA | 577 | G | OP1-P-O3' | 5.26 | 116.76 | 105.20 |
| 1 | BA | 1397 | C | N3-C2-O2 | -5.26 | 118.22 | 121.90 |
| 53 | DA | 964 | C | C2-N3-C4 | 5.26 | 122.53 | 119.90 |
| 53 | DA | 513 | A | OP2-P-O3' | 5.25 | 116.76 | 105.20 |
| 26 | CE | 88 | ARG | CA-CB-CG | 5.25 | 124.95 | 113.40 |
| 53 | DA | 997 | G | N1-C6-O6 | -5.25 | 116.75 | 119.90 |
| 41 | CU | 3 | ARG | CB-CA-C | 5.24 | 120.88 | 110.40 |
| 53 | DA | 990 | A | OP1-P-OP2 | -5.24 | 111.74 | 119.60 |
| 54 | DD | 124 | ARG | NE-CZ-NH2 | -5.24 | 117.68 | 120.30 |
| 53 | DA | 2613 | U | N3-C2-O2 | -5.24 | 118.53 | 122.20 |
| 53 | DA | 2263 | C | N3-C4-N4 | -5.23 | 114.34 | 118.00 |
| 53 | DA | 208 | C | N1-C2-O2 | 5.23 | 122.04 | 118.90 |
| 53 | DA | 26 | G | N3-C4-C5 | 5.23 | 131.22 | 128.60 |
| 53 | DA | 2723 | C | C6-N1-C2 | -5.23 | 118.21 | 120.30 |
| 1 | BA | 1211 | U | P-O3'-C3' | 5.23 | 125.97 | 119.70 |
| 22 | CA | 512 | G | O4'-C1'-N9 | 5.23 | 112.38 | 108.20 |
| 5 | BE | 15 | LEU | CA-CB-CG | 5.23 | 127.32 | 115.30 |
| 53 | DA | 1000 | A | C8-N9-C4 | 5.22 | 107.89 | 105.80 |
| 53 | DA | 2274 | A | OP2-P-O3' | 5.22 | 116.69 | 105.20 |
| 53 | DA | 586 | A | N9-C4-C5 | 5.22 | 107.89 | 105.80 |
| 53 | DA | 2295 | C | O5'-P-OP2 | -5.22 | 101.00 | 105.70 |
| 53 | DA | 2570 | G | N1-C6-O6 | -5.22 | 116.77 | 119.90 |
| 53 | DA | 1661 | G | N9-C4-C5 | 5.21 | 107.49 | 105.40 |
| 53 | DA | 2851 | A | O5'-P-OP2 | -5.21 | 101.01 | 105.70 |
| 53 | DA | 207 | A | OP2-P-O3' | 5.21 | 116.67 | 105.20 |
| 1 | BA | 330 | C | N3-C2-O2 | -5.21 | 118.25 | 121.90 |
| 53 | DA | 1026 | G | O5'-P-OP2 | 5.21 | 116.95 | 110.70 |
| 53 | DA | 2802 | G | N3-C4-N9 | -5.21 | 122.87 | 126.00 |
| 53 | DA | 1022 | G | N9-C4-C5 | 5.21 | 107.48 | 105.40 |
| 53 | DA | 1202 | G | N1-C6-O6 | -5.20 | 116.78 | 119.90 |
| 41 | CU | 3 | ARG | CA-CB-CG | 5.20 | 124.84 | 113.40 |
| 53 | DA | 2756 | U | C5-C4-O4 | 5.20 | 129.02 | 125.90 |
| 53 | DA | 422 | A | O5'-P-OP2 | 5.20 | 116.94 | 110.70 |
| 53 | DA | 570 | G | N3-C4-N9 | 5.19 | 129.12 | 126.00 |
| 53 | DA | 1146 | C | O5'-P-OP2 | -5.19 | 101.03 | 105.70 |
| 53 | DA | 522 | A | C5-N7-C8 | -5.19 | 101.30 | 103.90 |
| 53 | DA | 2582 | G | N3-C2-N2 | 5.19 | 123.53 | 119.90 |
| 22 | CA | 1779 | U | N1-C2-N3 | 5.19 | 118.02 | 114.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 53 | DA | 965 | C | N3-C4-C5 | 5.19 | 123.98 | 121.90 |
| 53 | DA | 1669 | A | C6-N1-C2 | -5.19 | 115.48 | 118.60 |
| 1 | AA | 792 | A | O4'-C1'-N9 | 5.19 | 112.35 | 108.20 |
| 53 | DA | 980 | A | O5'-P-OP1 | -5.19 | 101.03 | 105.70 |
| 53 | DA | 1020 | A | N9-C4-C5 | -5.19 | 103.72 | 105.80 |
| 23 | DB | 99 | A | C2-N3-C4 | -5.19 | 108.00 | 110.60 |
| 53 | DA | 563 | A | O5'-P-OP1 | -5.19 | 101.03 | 105.70 |
| 53 | DA | 946 | C | C6-N1-C2 | -5.19 | 118.22 | 120.30 |
| 53 | DA | 562 | U | N3-C2-O2 | -5.18 | 118.57 | 122.20 |
| 22 | CA | 818 | G | O3'-P-O5' | 5.18 | 113.85 | 104.00 |
| 53 | DA | 28 | A | OP2-P-O3' | 5.18 | 116.60 | 105.20 |
| 53 | DA | 995 | C | O4'-C1'-N1 | -5.18 | 104.06 | 108.20 |
| 53 | DA | 784 | G | P-O3'-C3' | 5.18 | 125.91 | 119.70 |
| 53 | DA | 1698 | A | C6-C5-N7 | -5.18 | 128.68 | 132.30 |
| 53 | DA | 2810 | A | O5'-P-OP2 | -5.18 | 101.04 | 105.70 |
| 53 | DA | 1760 | C | C6-N1-C2 | 5.18 | 122.37 | 120.30 |
| 53 | DA | 2499 | C | N1-C2-N3 | 5.18 | 122.82 | 119.20 |
| 53 | DA | 1888 | G | O5'-P-OP2 | -5.17 | 101.04 | 105.70 |
| 1 | AA | 328 | C | C2-N1-C1' | 5.17 | 124.49 | 118.80 |
| 53 | DA | 2814 | A | OP1-P-OP2 | 5.17 | 127.36 | 119.60 |
| 1 | BA | 330 | C | N3-C4-N4 | -5.17 | 114.38 | 118.00 |
| 1 | BA | 73 | C | O4'-C1'-N1 | 5.17 | 112.33 | 108.20 |
| 53 | DA | 1168 | G | C2-N3-C4 | -5.16 | 109.32 | 111.90 |
| 53 | DA | 1252 | G | O5'-P-OP1 | -5.16 | 101.05 | 105.70 |
| 53 | DA | 1930 | G | N3-C4-N9 | -5.16 | 122.90 | 126.00 |
| 1 | BA | 1492 | A | P-O3'-C3' | 5.16 | 125.89 | 119.70 |
| 1 | BA | 452 | A | C5-N7-C8 | -5.16 | 101.32 | 103.90 |
| 22 | CA | 404 | A | P-O3'-C3' | 5.16 | 125.89 | 119.70 |
| 22 | CA | 2585 | U | N1-C2-O2 | 5.16 | 126.41 | 122.80 |
| 53 | DA | 2724 | U | O5'-P-OP2 | -5.16 | 101.06 | 105.70 |
| 5 | BE | 122 | ASN | N-CA-C | 5.16 | 124.92 | 111.00 |
| 22 | CA | 271 | G | P-O3'-C3' | 5.16 | 125.89 | 119.70 |
| 22 | CA | 1730 | C | C6-N1-C2 | -5.16 | 118.24 | 120.30 |
| 53 | DA | 2062 | A | OP2-P-O3' | 5.16 | 116.54 | 105.20 |
| 53 | DA | 2756 | U | N3-C2-O2 | -5.16 | 118.59 | 122.20 |
| 53 | DA | 1927 | A | N1-C6-N6 | -5.15 | 115.51 | 118.60 |
| 1 | BA | 842 | U | C6-N1-C2 | -5.15 | 117.91 | 121.00 |
| 53 | DA | 494 | G | C8-N9-C4 | 5.15 | 108.46 | 106.40 |
| 1 | AA | 1286 | U | C2-N1-C1' | 5.14 | 123.87 | 117.70 |
| 1 | BA | 328 | C | N3-C2-O2 | -5.14 | 118.30 | 121.90 |
| 53 | DA | 1220 | G | N3-C2-N2 | 5.14 | 123.50 | 119.90 |
| 1 | BA | 1168 | U | C5-C6-N1 | 5.14 | 125.27 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 53 | DA | 970 | U | O5'-P-OP2 | -5.14 | 101.07 | 105.70 |
| 53 | DA | 2435 | A | O5'-P-OP1 | -5.14 | 101.07 | 105.70 |
| 12 | BL | 121 | ARG | NE-CZ-NH1 | 5.14 | 122.87 | 120.30 |
| 53 | DA | 1659 | G | C8-N9-C1' | 5.14 | 133.68 | 127.00 |
| 1 | BA | 1003 | G | C8-N9-C1' | -5.13 | 120.33 | 127.00 |
| 1 | BA | 1322 | C | C2-N1-C1' | 5.13 | 124.45 | 118.80 |
| 22 | CA | 653 | U | C5-C6-N1 | 5.13 | 125.27 | 122.70 |
| 1 | BA | 1322 | C | N1-C2-O2 | 5.13 | 121.98 | 118.90 |
| 53 | DA | 2020 | A | OP2-P-O3' | 5.13 | 116.49 | 105.20 |
| 53 | DA | 929 | U | N1-C2-O2 | -5.13 | 119.21 | 122.80 |
| 53 | DA | 845 | A | N1-C6-N6 | 5.12 | 121.67 | 118.60 |
| 53 | DA | 2812 | G | N3-C4-C5 | 5.12 | 131.16 | 128.60 |
| 53 | DA | 1788 | C | N3-C4-N4 | 5.12 | 121.58 | 118.00 |
| 53 | DA | 1849 | G | N3-C2-N2 | -5.11 | 116.32 | 119.90 |
| 53 | DA | 2838 | G | OP2-P-O3' | 5.11 | 116.45 | 105.20 |
| 53 | DA | 433 | C | N1-C2-O2 | -5.11 | 115.83 | 118.90 |
| 53 | DA | 298 | G | C5-C6-O6 | -5.11 | 125.54 | 128.60 |
| 53 | DA | 503 | A | C8-N9-C4 | -5.11 | 103.76 | 105.80 |
| 53 | DA | 2487 | G | OP2-P-O3' | 5.11 | 116.43 | 105.20 |
| 53 | DA | 2439 | A | C4-C5-C6 | 5.10 | 119.55 | 117.00 |
| 53 | DA | 465 | G | C6-N1-C2 | 5.10 | 128.16 | 125.10 |
| 53 | DA | 752 | A | N1-C6-N6 | -5.10 | 115.54 | 118.60 |
| 1 | AA | 5 | U | C5-C6-N1 | 5.09 | 125.25 | 122.70 |
| 53 | DA | 202 | U | C5-C4-O4 | 5.09 | 128.95 | 125.90 |
| 53 | DA | 372 | G | O5'-P-OP2 | 5.09 | 116.81 | 110.70 |
| 22 | CA | 140 | C | C2-N1-C1' | 5.09 | 124.40 | 118.80 |
| 22 | CA | 2071 | A | O3'-P-O5' | -5.09 | 94.33 | 104.00 |
| 53 | DA | 561 | G | C5-N7-C8 | -5.09 | 101.76 | 104.30 |
| 53 | DA | 1160 | G | N9-C4-C5 | 5.09 | 107.44 | 105.40 |
| 53 | DA | 2775 | G | OP2-P-O3' | 5.09 | 116.39 | 105.20 |
| 53 | DA | 8 | C | C6-N1-C2 | -5.08 | 118.27 | 120.30 |
| 22 | CA | 185 | G | C8-N9-C4 | -5.08 | 104.37 | 106.40 |
| 53 | DA | 969 | G | N9-C4-C5 | -5.08 | 103.37 | 105.40 |
| 53 | DA | 1429 | G | N1-C6-O6 | -5.08 | 116.85 | 119.90 |
| 53 | DA | 1936 | A | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 8 | BH | 59 | LEU | CA-CB-CG | 5.08 | 126.97 | 115.30 |
| 53 | DA | 2391 | G | O4'-C1'-N9 | 5.08 | 112.26 | 108.20 |
| 53 | DA | 2448 | A | N9-C4-C5 | 5.08 | 107.83 | 105.80 |
| 35 | CO | 101 | GLY | N-CA-C | 5.07 | 125.78 | 113.10 |
| 53 | DA | 943 | A | C2-N3-C4 | -5.07 | 108.06 | 110.60 |
| 53 | DA | 1651 | G | C8-N9-C4 | -5.07 | 104.37 | 106.40 |
| 53 | DA | 2429[A] | G | C4-N9-C1' | -5.07 | 119.91 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|---------|------|------------|-------|-------------|----------|
| 53 | DA | 2429[B] | G | C4-N9-C1' | -5.07 | 119.91 | 126.50 |
| 53 | DA | 2492 | U | C5-C6-N1 | 5.07 | 125.24 | 122.70 |
| 1 | AA | 858 | G | N3-C4-N9 | 5.07 | 129.04 | 126.00 |
| 1 | BA | 530 | G | C8-N9-C1' | -5.07 | 120.41 | 127.00 |
| 22 | CA | 60 | G | C4-N9-C1' | -5.07 | 119.91 | 126.50 |
| 53 | DA | 811 | U | C5-C4-O4 | 5.07 | 128.94 | 125.90 |
| 1 | BA | 572 | A | O3'-P-O5' | 5.06 | 113.61 | 104.00 |
| 22 | CA | 757 | G | N1-C6-O6 | 5.06 | 122.94 | 119.90 |
| 53 | DA | 837 | C | C2-N3-C4 | -5.06 | 117.37 | 119.90 |
| 53 | DA | 969 | G | C4-C5-N7 | 5.06 | 112.82 | 110.80 |
| 53 | DA | 2887[A] | A | N1-C6-N6 | 5.06 | 121.63 | 118.60 |
| 53 | DA | 2887[B] | A | N1-C6-N6 | 5.06 | 121.63 | 118.60 |
| 22 | CA | 1340 | U | C2-N1-C1' | 5.05 | 123.76 | 117.70 |
| 22 | CA | 974 | G | C4-C5-N7 | 5.05 | 112.82 | 110.80 |
| 53 | DA | 1328 | A | OP2-P-O3' | 5.05 | 116.31 | 105.20 |
| 53 | DA | 2684 | U | C6-N1-C2 | -5.05 | 117.97 | 121.00 |
| 53 | DA | 1674 | G | O4'-C1'-N9 | -5.05 | 104.16 | 108.20 |
| 1 | AA | 1222 | G | C5-C6-O6 | -5.05 | 125.57 | 128.60 |
| 53 | DA | 102 | U | C6-N1-C1' | -5.05 | 114.13 | 121.20 |
| 23 | DB | 93 | C | N3-C4-C5 | 5.05 | 123.92 | 121.90 |
| 53 | DA | 506 | G | C2-N3-C4 | -5.04 | 109.38 | 111.90 |
| 53 | DA | 468 | G | C2-N3-C4 | -5.04 | 109.38 | 111.90 |
| 1 | AA | 1279 | G | C6-C5-N7 | -5.04 | 127.38 | 130.40 |
| 53 | DA | 1267 | U | N1-C2-O2 | -5.04 | 119.28 | 122.80 |
| 1 | BA | 27 | G | C5-C6-O6 | -5.03 | 125.58 | 128.60 |
| 1 | BA | 468 | A | C8-N9-C4 | -5.03 | 103.79 | 105.80 |
| 53 | DA | 1698 | A | N1-C6-N6 | 5.03 | 121.62 | 118.60 |
| 53 | DA | 749 | A | O5'-P-OP2 | -5.03 | 101.17 | 105.70 |
| 53 | DA | 1930 | G | N3-C2-N2 | -5.03 | 116.38 | 119.90 |
| 1 | BA | 211 | G | N3-C4-C5 | -5.03 | 126.09 | 128.60 |
| 53 | DA | 1816 | C | N1-C2-O2 | -5.03 | 115.88 | 118.90 |
| 22 | CA | 135 | U | C5-C6-N1 | 5.02 | 125.21 | 122.70 |
| 53 | DA | 2684 | U | O5'-P-OP2 | -5.02 | 101.18 | 105.70 |
| 53 | DA | 663 | G | N3-C2-N2 | -5.02 | 116.38 | 119.90 |
| 22 | CA | 741 | U | N3-C2-O2 | 5.02 | 125.72 | 122.20 |
| 53 | DA | 1605 | C | N3-C2-O2 | 5.02 | 125.41 | 121.90 |
| 53 | DA | 2810 | A | OP1-P-OP2 | 5.02 | 127.13 | 119.60 |
| 1 | BA | 479 | U | C5-C6-N1 | 5.02 | 125.21 | 122.70 |
| 53 | DA | 1905 | C | N3-C4-N4 | -5.02 | 114.49 | 118.00 |
| 53 | DA | 2782 | G | C4-N9-C1' | 5.02 | 133.02 | 126.50 |
| 53 | DA | 2008 | C | N3-C4-N4 | 5.01 | 121.51 | 118.00 |
| 53 | DA | 2055 | C | N1-C2-O2 | -5.01 | 115.89 | 118.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 53 | DA | 1964 | G | O4'-C1'-N9 | -5.01 | 104.19 | 108.20 |
| 53 | DA | 1208 | C | N1-C2-O2 | 5.01 | 121.91 | 118.90 |
| 1 | BA | 1499 | A | N1-C6-N6 | 5.01 | 121.60 | 118.60 |
| 23 | DB | 72 | G | C2-N3-C4 | -5.00 | 109.40 | 111.90 |
| 53 | DA | 530 | G | N1-C6-O6 | 5.00 | 122.90 | 119.90 |
| 53 | DA | 1790 | C | N3-C4-N4 | 5.00 | 121.50 | 118.00 |
| 53 | DA | 2722 | G | N3-C2-N2 | -5.00 | 116.40 | 119.90 |

There are no chirality outliers.

All (10) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | BA | 702 | A | Sidechain |
| 6 | BF | 90 | MET | Peptide |
| 47 | C0 | 3 | LYS | Peptide |
| 25 | CD | 151 | THR | Peptide |
| 30 | CJ | 98 | VAL | Peptide |
| 32 | CL | 34 | GLY | Peptide |
| 47 | D0 | 3[B] | LYS | Peptide |
| 24 | DC | 232 | HIS | Peptide |
| 55 | DI | 67 | THR | Peptide |
| 30 | DJ | 98 | VAL | Peptide |

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AA | 32930 | 0 | 16591 | 191 | 0 |
| 1 | BA | 32908 | 0 | 16580 | 233 | 0 |
| 2 | AB | 1753 | 0 | 1780 | 26 | 0 |
| 2 | BB | 1753 | 0 | 1780 | 28 | 0 |
| 3 | AC | 1625 | 0 | 1696 | 15 | 0 |
| 3 | BC | 1625 | 0 | 1696 | 35 | 0 |
| 4 | AD | 1643 | 0 | 1707 | 20 | 0 |
| 4 | BD | 1643 | 0 | 1707 | 17 | 0 |
| 5 | AE | 1144 | 0 | 1185 | 28 | 0 |
| 5 | BE | 1105 | 0 | 1148 | 59 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6 | AF | 862 | 0 | 864 | 9 | 0 |
| 6 | BF | 817 | 0 | 808 | 22 | 0 |
| 7 | AG | 1182 | 0 | 1238 | 21 | 0 |
| 7 | BG | 1182 | 0 | 1238 | 33 | 0 |
| 8 | AH | 979 | 0 | 1031 | 18 | 0 |
| 8 | BH | 979 | 0 | 1031 | 18 | 0 |
| 9 | AI | 1022 | 0 | 1070 | 27 | 0 |
| 9 | BI | 1022 | 0 | 1070 | 24 | 0 |
| 10 | AJ | 796 | 0 | 836 | 40 | 0 |
| 10 | BJ | 787 | 0 | 828 | 20 | 0 |
| 11 | AK | 877 | 0 | 887 | 14 | 0 |
| 11 | BK | 877 | 0 | 887 | 28 | 0 |
| 12 | AL | 957 | 0 | 1017 | 9 | 0 |
| 12 | BL | 957 | 0 | 1017 | 21 | 0 |
| 13 | AM | 884 | 0 | 941 | 33 | 0 |
| 13 | BM | 884 | 0 | 941 | 24 | 0 |
| 14 | AN | 805 | 0 | 844 | 28 | 0 |
| 14 | BN | 805 | 0 | 844 | 40 | 0 |
| 15 | AO | 714 | 0 | 734 | 8 | 0 |
| 15 | BO | 714 | 0 | 734 | 23 | 0 |
| 16 | AP | 649 | 0 | 666 | 5 | 0 |
| 16 | BP | 649 | 0 | 666 | 10 | 0 |
| 17 | AQ | 649 | 0 | 691 | 9 | 0 |
| 17 | BQ | 649 | 0 | 691 | 21 | 0 |
| 18 | AR | 456 | 0 | 478 | 6 | 0 |
| 18 | BR | 456 | 0 | 478 | 13 | 0 |
| 19 | AS | 638 | 0 | 665 | 15 | 0 |
| 19 | BS | 638 | 0 | 665 | 28 | 0 |
| 20 | AT | 670 | 0 | 719 | 12 | 0 |
| 20 | BT | 665 | 0 | 714 | 13 | 0 |
| 21 | AU | 465 | 0 | 491 | 9 | 0 |
| 21 | BU | 465 | 0 | 491 | 8 | 0 |
| 22 | CA | 62229 | 0 | 31319 | 410 | 0 |
| 23 | CB | 2529 | 0 | 1281 | 12 | 0 |
| 23 | DB | 2569 | 0 | 1301 | 9 | 0 |
| 24 | CC | 2083 | 0 | 2154 | 37 | 0 |
| 24 | DC | 2083 | 0 | 2154 | 15 | 0 |
| 25 | CD | 1565 | 0 | 1616 | 30 | 0 |
| 26 | CE | 1552 | 0 | 1619 | 26 | 0 |
| 26 | DE | 1552 | 0 | 1619 | 3 | 0 |
| 27 | CF | 1411 | 0 | 1444 | 22 | 0 |
| 27 | DF | 1411 | 0 | 1444 | 19 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28 | CG | 1323 | 0 | 1371 | 9 | 0 |
| 28 | DG | 1323 | 0 | 1371 | 6 | 0 |
| 29 | CH | 1110 | 0 | 1148 | 13 | 0 |
| 29 | DH | 1110 | 0 | 1148 | 13 | 0 |
| 30 | CJ | 979 | 0 | 1028 | 24 | 0 |
| 30 | DJ | 979 | 0 | 1028 | 28 | 0 |
| 31 | CK | 1129 | 0 | 1162 | 16 | 0 |
| 31 | DK | 1129 | 0 | 1162 | 5 | 0 |
| 32 | CL | 938 | 0 | 1012 | 21 | 0 |
| 32 | DL | 946 | 0 | 1023 | 11 | 0 |
| 33 | CM | 1053 | 0 | 1129 | 31 | 0 |
| 33 | DM | 1053 | 0 | 1129 | 11 | 0 |
| 34 | CN | 1075 | 0 | 1155 | 6 | 0 |
| 34 | DN | 1092 | 0 | 1179 | 10 | 0 |
| 35 | CO | 960 | 0 | 1000 | 17 | 0 |
| 35 | DO | 993 | 0 | 1034 | 6 | 0 |
| 36 | CP | 892 | 0 | 923 | 15 | 0 |
| 36 | DP | 900 | 0 | 935 | 9 | 0 |
| 37 | CQ | 917 | 0 | 962 | 7 | 0 |
| 37 | DQ | 917 | 0 | 962 | 9 | 0 |
| 38 | CR | 947 | 0 | 1019 | 23 | 0 |
| 38 | DR | 947 | 0 | 1019 | 12 | 0 |
| 39 | CS | 816 | 0 | 839 | 9 | 0 |
| 39 | DS | 816 | 0 | 839 | 7 | 0 |
| 40 | CT | 857 | 0 | 922 | 6 | 0 |
| 40 | DT | 857 | 0 | 922 | 3 | 0 |
| 41 | CU | 739 | 0 | 807 | 18 | 0 |
| 41 | DU | 739 | 0 | 807 | 12 | 0 |
| 42 | CV | 780 | 0 | 831 | 26 | 0 |
| 42 | DV | 780 | 0 | 831 | 4 | 0 |
| 43 | CW | 753 | 0 | 780 | 7 | 0 |
| 43 | DW | 753 | 0 | 780 | 2 | 0 |
| 44 | CX | 569 | 0 | 581 | 7 | 0 |
| 44 | DX | 591 | 0 | 606 | 4 | 0 |
| 45 | CY | 625 | 0 | 652 | 11 | 0 |
| 45 | DY | 625 | 0 | 652 | 2 | 0 |
| 46 | CZ | 501 | 0 | 531 | 10 | 0 |
| 46 | DZ | 501 | 0 | 531 | 4 | 0 |
| 47 | C0 | 449 | 0 | 488 | 2 | 0 |
| 47 | D0 | 463 | 0 | 504 | 1 | 0 |
| 48 | C1 | 444 | 0 | 458 | 12 | 0 |
| 48 | D1 | 444 | 0 | 458 | 6 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 49 | C2 | 409 | 0 | 440 | 6 | 0 |
| 49 | D2 | 414 | 0 | 442 | 8 | 0 |
| 50 | C3 | 377 | 0 | 418 | 14 | 0 |
| 50 | D3 | 377 | 0 | 418 | 7 | 0 |
| 51 | C4 | 504 | 0 | 572 | 10 | 0 |
| 51 | D4 | 504 | 0 | 572 | 5 | 0 |
| 52 | C5 | 302 | 0 | 340 | 7 | 0 |
| 52 | D5 | 302 | 0 | 340 | 0 | 0 |
| 53 | DA | 62361 | 0 | 31381 | 308 | 0 |
| 54 | DD | 1576 | 0 | 1627 | 14 | 0 |
| 55 | DI | 1023 | 0 | 1052 | 20 | 0 |
| 56 | AA | 70 | 0 | 0 | 0 | 0 |
| 56 | BA | 41 | 0 | 0 | 0 | 0 |
| 56 | C3 | 1 | 0 | 0 | 0 | 0 |
| 56 | CA | 155 | 0 | 0 | 0 | 0 |
| 56 | CB | 3 | 0 | 0 | 0 | 0 |
| 56 | DA | 183 | 0 | 0 | 0 | 0 |
| 56 | DB | 9 | 0 | 0 | 0 | 0 |
| 56 | DR | 1 | 0 | 0 | 0 | 0 |
| 57 | AA | 13 | 0 | 18 | 1 | 0 |
| 57 | BA | 13 | 0 | 18 | 2 | 0 |
| 57 | DA | 26 | 0 | 36 | 8 | 0 |
| 57 | DQ | 13 | 0 | 18 | 3 | 0 |
| 57 | DR | 13 | 0 | 18 | 10 | 0 |
| 57 | DS | 13 | 0 | 18 | 2 | 0 |
| 58 | AA | 16 | 0 | 28 | 0 | 0 |
| 58 | DA | 40 | 0 | 70 | 5 | 0 |
| 58 | DE | 16 | 0 | 28 | 0 | 0 |
| 58 | DK | 8 | 0 | 14 | 0 | 0 |
| 58 | DN | 8 | 0 | 14 | 6 | 0 |
| 58 | DS | 8 | 0 | 14 | 0 | 0 |
| 58 | DT | 16 | 0 | 28 | 0 | 0 |
| 59 | AA | 24 | 0 | 48 | 1 | 0 |
| 59 | DA | 66 | 0 | 132 | 16 | 0 |
| 59 | DM | 6 | 0 | 12 | 0 | 0 |
| 60 | AB | 1 | 0 | 0 | 0 | 0 |
| 60 | C5 | 1 | 0 | 0 | 0 | 0 |
| 60 | D5 | 1 | 0 | 0 | 0 | 0 |
| 61 | AL | 7 | 0 | 10 | 0 | 0 |
| 61 | D3 | 7 | 0 | 10 | 5 | 0 |
| 61 | DA | 42 | 0 | 60 | 3 | 0 |
| 61 | DL | 7 | 0 | 10 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 61 | DP | 7 | 0 | 10 | 4 | 0 |
| 61 | DQ | 7 | 0 | 10 | 1 | 0 |
| 62 | DA | 40 | 0 | 76 | 7 | 0 |
| 63 | DA | 32 | 0 | 44 | 4 | 0 |
| 64 | D1 | 10 | 0 | 14 | 0 | 0 |
| 64 | D3 | 10 | 0 | 14 | 0 | 0 |
| 64 | DA | 50 | 0 | 70 | 3 | 0 |
| 64 | DS | 10 | 0 | 14 | 0 | 0 |
| 64 | DU | 10 | 0 | 14 | 1 | 0 |
| 65 | DA | 12 | 0 | 9 | 1 | 0 |
| 66 | D0 | 4 | 0 | 6 | 0 | 0 |
| 66 | D1 | 4 | 0 | 6 | 0 | 0 |
| 66 | DA | 24 | 0 | 36 | 11 | 0 |
| 66 | DB | 12 | 0 | 18 | 1 | 0 |
| 66 | DR | 4 | 0 | 6 | 0 | 0 |
| 67 | DA | 11 | 0 | 5 | 1 | 0 |
| 68 | DA | 8 | 0 | 12 | 0 | 0 |
| 69 | AA | 509 | 0 | 0 | 9 | 0 |
| 69 | AC | 6 | 0 | 0 | 0 | 0 |
| 69 | AD | 2 | 0 | 0 | 0 | 0 |
| 69 | AE | 5 | 0 | 0 | 0 | 0 |
| 69 | AF | 1 | 0 | 0 | 0 | 0 |
| 69 | AG | 1 | 0 | 0 | 0 | 0 |
| 69 | AH | 1 | 0 | 0 | 0 | 0 |
| 69 | AJ | 2 | 0 | 0 | 0 | 0 |
| 69 | AK | 6 | 0 | 0 | 0 | 0 |
| 69 | AL | 10 | 0 | 0 | 1 | 0 |
| 69 | AM | 4 | 0 | 0 | 0 | 0 |
| 69 | AN | 6 | 0 | 0 | 2 | 0 |
| 69 | AO | 2 | 0 | 0 | 0 | 0 |
| 69 | AP | 2 | 0 | 0 | 2 | 0 |
| 69 | AS | 1 | 0 | 0 | 0 | 0 |
| 69 | AT | 2 | 0 | 0 | 0 | 0 |
| 69 | AU | 2 | 0 | 0 | 0 | 0 |
| 69 | BA | 286 | 0 | 0 | 16 | 0 |
| 69 | BD | 12 | 0 | 0 | 0 | 0 |
| 69 | BE | 1 | 0 | 0 | 0 | 0 |
| 69 | BF | 2 | 0 | 0 | 0 | 0 |
| 69 | BL | 5 | 0 | 0 | 1 | 0 |
| 69 | BN | 3 | 0 | 0 | 0 | 0 |
| 69 | BO | 1 | 0 | 0 | 0 | 0 |
| 69 | BP | 3 | 0 | 0 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 69 | BT | 5 | 0 | 0 | 0 | 0 |
| 69 | BU | 2 | 0 | 0 | 0 | 0 |
| 69 | C3 | 2 | 0 | 0 | 1 | 0 |
| 69 | C4 | 1 | 0 | 0 | 0 | 0 |
| 69 | CA | 692 | 0 | 0 | 56 | 0 |
| 69 | CB | 13 | 0 | 0 | 1 | 0 |
| 69 | CC | 8 | 0 | 0 | 0 | 0 |
| 69 | CD | 6 | 0 | 0 | 0 | 0 |
| 69 | CE | 6 | 0 | 0 | 2 | 0 |
| 69 | CK | 1 | 0 | 0 | 0 | 0 |
| 69 | CL | 1 | 0 | 0 | 1 | 0 |
| 69 | CM | 5 | 0 | 0 | 0 | 0 |
| 69 | CO | 1 | 0 | 0 | 0 | 0 |
| 69 | CS | 1 | 0 | 0 | 0 | 0 |
| 69 | CU | 2 | 0 | 0 | 1 | 0 |
| 69 | CV | 2 | 0 | 0 | 0 | 0 |
| 69 | CW | 1 | 0 | 0 | 0 | 0 |
| 69 | CY | 1 | 0 | 0 | 0 | 0 |
| 69 | D0 | 25 | 0 | 0 | 0 | 0 |
| 69 | D1 | 47 | 0 | 0 | 3 | 0 |
| 69 | D2 | 9 | 0 | 0 | 1 | 0 |
| 69 | D3 | 25 | 0 | 0 | 0 | 0 |
| 69 | D4 | 38 | 0 | 0 | 2 | 0 |
| 69 | D5 | 14 | 0 | 0 | 0 | 0 |
| 69 | DA | 4815 | 0 | 0 | 46 | 0 |
| 69 | DB | 209 | 0 | 0 | 2 | 0 |
| 69 | DC | 106 | 0 | 0 | 2 | 0 |
| 69 | DD | 103 | 0 | 0 | 1 | 0 |
| 69 | DE | 62 | 0 | 0 | 0 | 0 |
| 69 | DF | 14 | 0 | 0 | 1 | 0 |
| 69 | DG | 6 | 0 | 0 | 0 | 0 |
| 69 | DH | 2 | 0 | 0 | 0 | 0 |
| 69 | DK | 59 | 0 | 0 | 1 | 0 |
| 69 | DL | 45 | 0 | 0 | 1 | 0 |
| 69 | DM | 67 | 0 | 0 | 0 | 0 |
| 69 | DN | 74 | 0 | 0 | 0 | 0 |
| 69 | DO | 42 | 0 | 0 | 0 | 0 |
| 69 | DP | 37 | 0 | 0 | 1 | 0 |
| 69 | DQ | 27 | 0 | 0 | 2 | 0 |
| 69 | DR | 67 | 0 | 0 | 1 | 0 |
| 69 | DS | 50 | 0 | 0 | 2 | 0 |
| 69 | DT | 61 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 69 | DU | 19 | 0 | 0 | 0 | 0 |
| 69 | DV | 22 | 0 | 0 | 0 | 0 |
| 69 | DW | 32 | 0 | 0 | 1 | 0 |
| 69 | DX | 30 | 0 | 0 | 2 | 0 |
| 69 | DY | 10 | 0 | 0 | 1 | 0 |
| 69 | DZ | 8 | 0 | 0 | 0 | 0 |
| All | All | 295060 | 0 | 194384 | 2370 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (2370) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 14:BN:26:GLU:N | 14:BN:26:GLU:OE2 | 1.97 | 0.96 |
| 1:BA:1518:MA6:H103 | 1:BA:1519:MA6:H102 | 1.44 | 0.94 |
| 14:AN:64:CYS:SG | 69:AN:204:HOH:O | 2.25 | 0.94 |
| 1:AA:1518:MA6:H103 | 1:AA:1519:MA6:H102 | 1.50 | 0.94 |
| 22:CA:1652:A:OP1 | 35:CO:8:ARG:NH2 | 2.04 | 0.90 |
| 14:BN:23:LYS:N | 14:BN:26:GLU:OE1 | 2.04 | 0.90 |
| 22:CA:789:A:N1 | 69:CA:3287:HOH:O | 2.06 | 0.89 |
| 1:AA:702:A:N6 | 53:DA:1846:G:O2' | 2.05 | 0.89 |
| 53:DA:2885[B]:G:OP1 | 67:DA:3212:GUN:N2 | 2.06 | 0.89 |
| 11:AK:94:GLU:OE2 | 11:AK:98:ARG:NH2 | 2.06 | 0.89 |
| 5:BE:102:GLY:O | 5:BE:104:GLY:N | 2.05 | 0.88 |
| 53:DA:2116:G:O6 | 53:DA:2171:A:N6 | 2.06 | 0.88 |
| 11:AK:13:ARG:NH2 | 11:AK:77:TYR:OH | 2.07 | 0.88 |
| 1:AA:1130:A:OP1 | 9:AI:18:ARG:NH1 | 2.07 | 0.87 |
| 22:CA:878:A:N6 | 22:CA:899:A:O2' | 2.07 | 0.86 |
| 22:CA:2429:G:OP2 | 69:CA:3861:HOH:O | 1.91 | 0.86 |
| 1:BA:140:U:O2 | 1:BA:183:C:N4 | 2.10 | 0.85 |
| 22:CA:2430:A:OP2 | 69:CA:3861:HOH:O | 1.94 | 0.85 |
| 62:DA:3225:SPD:H92 | 62:DA:3225:SPD:H52 | 1.59 | 0.85 |
| 53:DA:1508:A:O2' | 53:DA:1509:A:O4' | 1.95 | 0.84 |
| 22:CA:459:U:O2' | 41:CU:73:ARG:NH2 | 2.10 | 0.84 |
| 1:BA:978:A:OP2 | 1:BA:1362:A:N6 | 2.10 | 0.84 |
| 53:DA:141:G:OP2 | 53:DA:142:A:N6 | 2.11 | 0.84 |
| 22:CA:2579:C:OP1 | 69:CA:3871:HOH:O | 1.96 | 0.83 |
| 53:DA:480:A:OP2 | 42:DV:44:LYS:NZ | 2.12 | 0.83 |
| 26:CE:170:ARG:NH1 | 26:CE:179:SER:OG | 2.13 | 0.81 |
| 1:BA:1147:C:O2 | 9:BI:18:ARG:NH2 | 2.14 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 14:BN:26:GLU:H | 14:BN:26:GLU:CD | 1.84 | 0.81 |
| 13:BM:11:ASP:OD1 | 13:BM:12:HIS:N | 2.14 | 0.81 |
| 14:AN:67:THR:N | 69:AN:204:HOH:O | 2.15 | 0.80 |
| 22:CA:2210:U:O2 | 69:CA:3787:HOH:O | 1.99 | 0.80 |
| 1:AA:127:G:O2' | 17:AQ:6:ARG:NH1 | 2.15 | 0.79 |
| 22:CA:734:A:N3 | 69:CA:3705:HOH:O | 2.14 | 0.79 |
| 53:DA:2224:G:OP1 | 24:DC:265:LYS:NZ | 2.15 | 0.79 |
| 38:DR:19:LYS:HD3 | 57:DR:202:PG4:H22 | 1.64 | 0.79 |
| 22:CA:250:G:OP2 | 51:C4:13:ARG:NH1 | 2.14 | 0.79 |
| 4:AD:100:ASN:OD1 | 4:AD:111:ARG:NH1 | 2.16 | 0.79 |
| 24:CC:258:ARG:NH1 | 24:CC:264:ASP:OD1 | 2.16 | 0.78 |
| 22:CA:1154:G:OP2 | 38:CR:58:ARG:NH1 | 2.16 | 0.78 |
| 9:BI:12:ARG:NH2 | 9:BI:107:ASP:OD2 | 2.16 | 0.78 |
| 38:DR:20:GLN:HG2 | 57:DR:202:PG4:H51 | 1.64 | 0.78 |
| 22:CA:2640:G:OP1 | 31:CK:95:ARG:NH1 | 2.17 | 0.78 |
| 4:BD:100:ASN:OD1 | 4:BD:111:ARG:NH1 | 2.16 | 0.78 |
| 22:CA:1508:A:O2' | 22:CA:1509:A:O4' | 2.01 | 0.78 |
| 7:AG:68:ASN:O | 7:AG:138:ARG:NH1 | 2.17 | 0.78 |
| 5:BE:151:GLU:O | 5:BE:154:ALA:HB3 | 1.84 | 0.77 |
| 15:BO:18:ASP:OD1 | 15:BO:19:ALA:N | 2.17 | 0.77 |
| 16:BP:1:MET:N | 16:BP:1:MET:SD | 2.53 | 0.77 |
| 53:DA:1236:G:N7 | 59:DA:3189:PUT:H41 | 2.00 | 0.77 |
| 1:AA:1147:C:O2 | 9:AI:18:ARG:NH2 | 2.18 | 0.76 |
| 1:BA:742:G:O6 | 69:BA:1865:HOH:O | 2.03 | 0.76 |
| 1:BA:842:U:H3' | 1:BA:843:U:C5' | 2.16 | 0.76 |
| 63:DA:3203:1PE:H221 | 69:DA:3975:HOH:O | 1.86 | 0.76 |
| 1:BA:1026:G:N1 | 1:BA:1035:A:N1 | 2.34 | 0.76 |
| 22:CA:2262:U:OP1 | 44:CX:41:ARG:NH2 | 2.19 | 0.76 |
| 25:CD:12:THR:OG1 | 25:CD:13:ARG:N | 2.17 | 0.76 |
| 7:AG:111:ARG:NH1 | 7:AG:123:GLU:OE2 | 2.19 | 0.75 |
| 39:DS:37:GLU:O | 69:DS:319:HOH:O | 2.03 | 0.75 |
| 23:DB:90:C:OP2 | 69:DB:319:HOH:O | 2.04 | 0.75 |
| 1:AA:1134:G:N2 | 1:AA:1140:C:N3 | 2.34 | 0.75 |
| 22:CA:77:G:O2' | 46:CZ:7:ARG:NH2 | 2.20 | 0.75 |
| 22:CA:2032:G:N7 | 69:CA:3866:HOH:O | 2.20 | 0.74 |
| 53:DA:1311:G:N7 | 69:DA:6065:HOH:O | 2.20 | 0.74 |
| 3:AC:40:ARG:NH1 | 3:AC:55:ILE:O | 2.21 | 0.74 |
| 1:BA:836:G:N7 | 69:BA:1920:HOH:O | 2.21 | 0.74 |
| 1:BA:1130:A:OP1 | 9:BI:18:ARG:NH1 | 2.21 | 0.74 |
| 16:BP:42:ILE:O | 16:BP:44:SER:N | 2.20 | 0.74 |
| 1:BA:319:G:N7 | 69:BA:1722:HOH:O | 2.20 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 13:AM:82:ASP:OD2 | 27:DF:112:ARG:NH2 | 2.20 | 0.73 |
| 22:CA:2134:A:N6 | 22:CA:2157:G:O2' | 2.21 | 0.73 |
| 38:DR:19:LYS:HD3 | 57:DR:202:PG4:H41 | 1.71 | 0.72 |
| 24:DC:251:GLN:NE2 | 69:DC:406:HOH:O | 2.21 | 0.72 |
| 53:DA:2827:C:O2 | 66:DA:3198:EDO:H21 | 1.89 | 0.72 |
| 1:BA:516:PSU:O2 | 69:BA:1970:HOH:O | 2.07 | 0.72 |
| 22:CA:1588:G:N3 | 69:CA:3746:HOH:O | 2.22 | 0.72 |
| 1:BA:1109:C:H2' | 1:BA:1110:A:H5'' | 1.72 | 0.71 |
| 16:BP:46:LYS:HD3 | 16:BP:47:GLU:H | 1.54 | 0.71 |
| 22:CA:2685:G:OP1 | 32:CL:78:ARG:NH2 | 2.22 | 0.71 |
| 22:CA:820:A:N1 | 69:CA:3772:HOH:O | 2.23 | 0.71 |
| 66:DA:3198:EDO:H12 | 64:DA:3204:PGE:H32 | 1.72 | 0.71 |
| 22:CA:732:C:OP2 | 69:CA:3273:HOH:O | 2.09 | 0.71 |
| 1:BA:1279:G:OP1 | 10:BJ:9:ARG:NH2 | 2.24 | 0.71 |
| 53:DA:2428:G:OP2 | 59:DA:3224:PUT:H11 | 1.89 | 0.71 |
| 53:DA:1027:A:N3 | 69:DA:6955:HOH:O | 2.23 | 0.71 |
| 8:BH:77:ARG:NE | 8:BH:79:SER:O | 2.24 | 0.71 |
| 1:BA:1204:A:OP2 | 69:BA:1817:HOH:O | 2.09 | 0.70 |
| 22:CA:568:U:H1' | 22:CA:2030:6MZ:H9C1 | 1.73 | 0.70 |
| 9:AI:12:ARG:NH2 | 9:AI:107:ASP:OD2 | 2.24 | 0.70 |
| 12:BL:14:ARG:HA | 12:BL:14:ARG:HH11 | 1.56 | 0.70 |
| 41:DU:2:ILE:HG22 | 41:DU:7:LEU:HD21 | 1.73 | 0.70 |
| 22:CA:1825:U:OP2 | 69:CA:3822:HOH:O | 2.09 | 0.70 |
| 30:DJ:113:LYS:O | 30:DJ:117:MET:N | 2.23 | 0.70 |
| 22:CA:1602:U:O4 | 69:CA:3603:HOH:O | 2.08 | 0.70 |
| 1:BA:1518:MA6:H103 | 1:BA:1519:MA6:C10 | 2.20 | 0.70 |
| 22:CA:2495:G:N7 | 69:CA:3681:HOH:O | 2.23 | 0.70 |
| 1:BA:1266:G:N2 | 1:BA:1269:A:OP2 | 2.24 | 0.70 |
| 22:CA:616:A:OP2 | 69:CA:3263:HOH:O | 2.08 | 0.70 |
| 22:CA:978:G:N7 | 69:CA:3501:HOH:O | 2.24 | 0.70 |
| 1:AA:1486:G:OP2 | 69:AA:1925:HOH:O | 2.08 | 0.70 |
| 1:AA:1518:MA6:H103 | 1:AA:1519:MA6:C10 | 2.21 | 0.70 |
| 5:BE:66:LYS:O | 5:BE:70:ASN:ND2 | 2.25 | 0.70 |
| 19:BS:36:ARG:NH2 | 19:BS:75:ALA:O | 2.25 | 0.70 |
| 22:CA:686:U:OP2 | 69:CA:3607:HOH:O | 2.08 | 0.69 |
| 22:CA:581:C:OP2 | 38:CR:33:ARG:NE | 2.25 | 0.69 |
| 22:CA:2134:A:OP2 | 22:CA:2157:G:N2 | 2.24 | 0.69 |
| 1:BA:9:G:H5' | 5:BE:108:GLY:HA3 | 1.74 | 0.69 |
| 22:CA:2268:A:OP1 | 69:CA:3440:HOH:O | 2.09 | 0.69 |
| 1:BA:842:U:H3' | 1:BA:843:U:H5' | 1.74 | 0.69 |
| 21:AU:31:GLU:OE2 | 21:AU:34:ARG:NH2 | 2.25 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 57:DR:202:PG4:H62 | 69:DR:359:HOH:O | 1.92 | 0.69 |
| 53:DA:568:U:H1' | 53:DA:2030:6MZ:H9C1 | 1.74 | 0.69 |
| 1:AA:964:A:OP1 | 69:AA:2195:HOH:O | 2.11 | 0.69 |
| 24:CC:69:ARG:O | 24:CC:189:ARG:NH2 | 2.26 | 0.69 |
| 30:CJ:113:LYS:O | 30:CJ:117:MET:N | 2.26 | 0.69 |
| 41:CU:3:ARG:NH2 | 41:CU:5:GLU:OE2 | 2.27 | 0.68 |
| 37:DQ:68:GLU:OE2 | 69:DQ:307:HOH:O | 2.10 | 0.68 |
| 53:DA:2609:U:C5 | 66:DA:3194:EDO:H12 | 2.28 | 0.68 |
| 53:DA:1311:G:O2' | 69:DA:6066:HOH:O | 2.09 | 0.68 |
| 11:BK:94:GLU:OE2 | 11:BK:98:ARG:NH2 | 2.25 | 0.68 |
| 22:CA:1962:5MC:HM53 | 69:CA:3753:HOH:O | 1.93 | 0.68 |
| 1:AA:845:A:O3' | 18:AR:48:ARG:NH2 | 2.25 | 0.68 |
| 53:DA:1176:U:H2' | 53:DA:1177:G:C8 | 2.27 | 0.68 |
| 53:DA:2428:G:N7 | 59:DA:3224:PUT:N1 | 2.42 | 0.68 |
| 53:DA:2310:C:OP1 | 69:DA:3597:HOH:O | 2.12 | 0.68 |
| 53:DA:2072:C:OP1 | 69:DA:3838:HOH:O | 2.11 | 0.68 |
| 5:BE:38:VAL:HG13 | 5:BE:117:VAL:HG21 | 1.75 | 0.68 |
| 53:DA:1167:C:OP2 | 69:DA:4751:HOH:O | 2.12 | 0.68 |
| 22:CA:2720:U:OP1 | 37:CQ:53:ARG:NH2 | 2.26 | 0.68 |
| 41:CU:5:GLU:HG3 | 46:CZ:22:LEU:HD13 | 1.75 | 0.68 |
| 29:DH:116:ARG:NH2 | 29:DH:133:GLN:OE1 | 2.27 | 0.68 |
| 23:DB:84:G:H21 | 66:DB:212:EDO:H11 | 1.59 | 0.68 |
| 32:CL:93:GLN:NE2 | 32:CL:111:LYS:O | 2.27 | 0.67 |
| 1:BA:1376:U:O4 | 7:BG:10:ARG:NH1 | 2.27 | 0.67 |
| 22:CA:1998:A:OP2 | 25:CD:141:ARG:NH2 | 2.27 | 0.67 |
| 1:AA:738:C:OP1 | 6:AF:2:ARG:NH2 | 2.27 | 0.67 |
| 1:AA:980:C:O3' | 14:AN:13:ARG:NH2 | 2.27 | 0.67 |
| 53:DA:2720:U:OP1 | 37:DQ:53:ARG:NH2 | 2.28 | 0.67 |
| 22:CA:1187:G:N7 | 69:CA:3493:HOH:O | 2.27 | 0.67 |
| 5:BE:101:GLU:O | 5:BE:103:THR:N | 2.28 | 0.67 |
| 41:CU:28:ASN:ND2 | 41:CU:91:GLN:OE1 | 2.28 | 0.67 |
| 22:CA:591:U:H1' | 51:C4:2:PRO:HD2 | 1.77 | 0.67 |
| 50:D3:32:ALA:CB | 61:D3:102:PEG:H12 | 2.25 | 0.67 |
| 1:AA:453:G:N7 | 59:AA:1673:PUT:H42 | 2.10 | 0.67 |
| 13:AM:4:ILE:O | 13:AM:6:GLY:N | 2.28 | 0.67 |
| 1:BA:1360:A:N7 | 69:BA:1815:HOH:O | 2.28 | 0.67 |
| 1:BA:439:U:H4' | 4:BD:121:LYS:HD2 | 1.77 | 0.66 |
| 22:CA:1250:G:OP2 | 33:CM:21:ARG:NH2 | 2.28 | 0.66 |
| 1:AA:412:A:H1' | 1:AA:413:G:H5' | 1.75 | 0.66 |
| 53:DA:2799:A:N7 | 69:DA:5142:HOH:O | 2.28 | 0.66 |
| 1:AA:806:C:H4' | 57:AA:1670:PG4:H11 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AC:19:ASN:ND2 | 14:AN:90:ARG:O | 2.28 | 0.66 |
| 7:AG:138:ARG:NH2 | 7:AG:139:GLU:OE2 | 2.29 | 0.66 |
| 53:DA:846:U:O2' | 53:DA:847:U:OP2 | 2.11 | 0.66 |
| 12:BL:49:LEU:O | 69:BL:203:HOH:O | 2.13 | 0.66 |
| 1:AA:536:C:OP1 | 69:AA:1765:HOH:O | 2.13 | 0.66 |
| 13:AM:4:ILE:O | 13:AM:7:ILE:N | 2.26 | 0.66 |
| 22:CA:733:G:OP1 | 69:CA:3711:HOH:O | 2.14 | 0.66 |
| 28:DG:101:ASN:ND2 | 28:DG:116:GLN:OE1 | 2.28 | 0.66 |
| 22:CA:1385:A:O2' | 22:CA:1396:U:O2 | 2.12 | 0.66 |
| 22:CA:2127:G:O2' | 22:CA:2173:A:N3 | 2.29 | 0.66 |
| 1:BA:1197:A:OP1 | 69:BA:1934:HOH:O | 2.12 | 0.66 |
| 1:AA:1486:G:OP1 | 69:AA:1920:HOH:O | 2.13 | 0.66 |
| 22:CA:998:C:OP2 | 38:CR:58:ARG:NH2 | 2.28 | 0.66 |
| 22:CA:1378:A:O2' | 22:CA:1380:G:N7 | 2.23 | 0.66 |
| 32:CL:38:ILE:O | 69:CL:201:HOH:O | 2.14 | 0.66 |
| 9:BI:22:LYS:O | 9:BI:62:ASP:N | 2.29 | 0.65 |
| 35:CO:69:ARG:O | 35:CO:71:ARG:N | 2.29 | 0.65 |
| 22:CA:1823:G:N7 | 69:CA:3872:HOH:O | 2.29 | 0.65 |
| 22:CA:1417:C:OP1 | 69:CA:3746:HOH:O | 2.13 | 0.65 |
| 1:BA:1033:G:N2 | 1:BA:1034:G:N3 | 2.45 | 0.65 |
| 53:DA:2127:G:O2' | 53:DA:2128:G:O4' | 2.13 | 0.65 |
| 53:DA:788:A:OP1 | 59:DA:3223:PUT:H42 | 1.97 | 0.65 |
| 25:CD:151:THR:O | 25:CD:153:GLY:N | 2.25 | 0.65 |
| 3:AC:179:ARG:NH1 | 3:AC:206:GLU:OE1 | 2.29 | 0.65 |
| 22:CA:450:G:O6 | 69:CA:3238:HOH:O | 2.11 | 0.65 |
| 1:BA:1361:G:N2 | 1:BA:1362:A:N7 | 2.45 | 0.65 |
| 1:AA:7:A:N6 | 5:AE:97:GLN:OE1 | 2.30 | 0.65 |
| 1:BA:450:G:O5' | 69:BA:1918:HOH:O | 2.14 | 0.65 |
| 53:DA:2017:U:O4 | 66:DA:3209:EDO:H22 | 1.97 | 0.65 |
| 1:AA:263:A:OP2 | 20:AT:74:ARG:NH1 | 2.29 | 0.65 |
| 50:C3:11:LYS:NZ | 69:C3:201:HOH:O | 2.29 | 0.65 |
| 22:CA:85:G:OP1 | 42:CV:7:ARG:N | 2.28 | 0.65 |
| 28:DG:104:ASN:ND2 | 28:DG:114:ASP:OD1 | 2.30 | 0.65 |
| 1:AA:771:G:N7 | 69:AA:1798:HOH:O | 2.30 | 0.65 |
| 1:BA:1028:C:O2' | 1:BA:1029:U:O5' | 2.13 | 0.65 |
| 1:BA:880:C:OP1 | 12:BL:9:ARG:NH2 | 2.30 | 0.65 |
| 1:BA:1220:G:OP1 | 19:BS:37:ARG:NH2 | 2.30 | 0.65 |
| 26:CE:125:SER:O | 26:CE:137:LYS:NZ | 2.29 | 0.65 |
| 62:DA:3225:SPD:H92 | 62:DA:3225:SPD:C5 | 2.27 | 0.65 |
| 64:DA:3218:PGE:O4 | 69:DA:7614:HOH:O | 2.14 | 0.65 |
| 5:BE:104:GLY:HA3 | 5:BE:122:ASN:HA | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:CA:528:A:OP1 | 69:CA:3840:HOH:O | 2.15 | 0.64 |
| 23:CB:5:U:O2' | 23:CB:27:C:O2 | 2.16 | 0.64 |
| 1:AA:8:A:C6 | 4:AD:206:LYS:HB3 | 2.32 | 0.64 |
| 53:DA:812:C:O2' | 38:DR:13:ARG:NH1 | 2.30 | 0.64 |
| 44:DX:39:ARG:NH1 | 69:DX:124:HOH:O | 2.30 | 0.64 |
| 22:CA:2430:A:OP1 | 69:CA:3859:HOH:O | 2.15 | 0.64 |
| 53:DA:2209:G:N3 | 69:DA:5103:HOH:O | 2.30 | 0.64 |
| 9:BI:84:THR:HG21 | 9:BI:103:PHE:HB3 | 1.79 | 0.64 |
| 2:BB:120:GLN:O | 2:BB:125:THR:N | 2.30 | 0.64 |
| 11:AK:119:ASN:OD1 | 21:AU:35:ARG:NH1 | 2.31 | 0.64 |
| 9:AI:22:LYS:O | 9:AI:62:ASP:N | 2.29 | 0.64 |
| 30:DJ:100:LYS:CB | 30:DJ:141:GLU:HB2 | 2.27 | 0.64 |
| 25:CD:85:ALA:O | 25:CD:87:GLY:N | 2.28 | 0.64 |
| 26:CE:76:PRO:HA | 26:CE:82:GLY:HA2 | 1.80 | 0.64 |
| 53:DA:2033:A:H5' | 69:DA:4744:HOH:O | 1.97 | 0.64 |
| 53:DA:139:U:O4 | 41:DU:2:ILE:HG13 | 1.98 | 0.64 |
| 30:CJ:100:LYS:CB | 30:CJ:141:GLU:HB2 | 2.28 | 0.64 |
| 8:AH:54:ASP:OD1 | 8:AH:55:THR:N | 2.30 | 0.64 |
| 1:BA:415:A:O2' | 53:DA:2152:G:N2 | 2.30 | 0.63 |
| 53:DA:2127:G:O2' | 53:DA:2128:G:O5' | 2.15 | 0.63 |
| 1:AA:845:A:O2' | 18:AR:48:ARG:NH2 | 2.31 | 0.63 |
| 53:DA:136:G:H1 | 53:DA:143:C:N4 | 1.96 | 0.63 |
| 3:BC:139:GLN:O | 3:BC:141:ALA:N | 2.31 | 0.63 |
| 1:BA:1183:U:O2' | 1:BA:1185:G:OP2 | 2.16 | 0.63 |
| 38:DR:20:GLN:HG3 | 57:DR:202:PG4:H42 | 1.80 | 0.63 |
| 19:AS:36:ARG:NH2 | 19:AS:75:ALA:O | 2.32 | 0.63 |
| 47:C0:40:ASP:OD1 | 47:C0:45:ARG:NH1 | 2.32 | 0.63 |
| 1:AA:928:G:O2' | 1:AA:1533:C:OP1 | 2.16 | 0.63 |
| 5:BE:154:ALA:HA | 5:BE:157:ARG:HB3 | 1.81 | 0.63 |
| 1:BA:1328:C:H5'' | 13:BM:28:THR:HG21 | 1.80 | 0.63 |
| 42:CV:74:ASN:O | 42:CV:76:ALA:N | 2.31 | 0.63 |
| 53:DA:1061:U:OP2 | 30:DJ:10:LYS:NZ | 2.31 | 0.63 |
| 37:CQ:113:ARG:O | 37:CQ:115:ASN:N | 2.31 | 0.63 |
| 1:AA:405:U:OP2 | 4:AD:3:ARG:NH1 | 2.32 | 0.63 |
| 1:BA:263:A:OP1 | 20:BT:74:ARG:NH1 | 2.31 | 0.62 |
| 22:CA:2031:A:C6 | 22:CA:2498:OMC:H1' | 2.34 | 0.62 |
| 22:CA:528:A:C2 | 22:CA:2043:C:H4' | 2.34 | 0.62 |
| 1:BA:1187:G:H5' | 9:BI:115:LYS:HE3 | 1.82 | 0.62 |
| 19:BS:29:LYS:HB3 | 19:BS:30:PRO:HD2 | 1.82 | 0.62 |
| 41:DU:1:MET:HE3 | 41:DU:1:MET:H1 | 1.64 | 0.62 |
| 30:DJ:100:LYS:HB2 | 30:DJ:141:GLU:HB2 | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 22:CA:2498:OMC:HM22 | 22:CA:2499:C:H5' | 1.82 | 0.62 |
| 26:CE:23:PHE:CD1 | 26:CE:111:GLU:HG3 | 2.35 | 0.62 |
| 46:CZ:45:GLN:O | 46:CZ:47:ARG:N | 2.28 | 0.62 |
| 53:DA:878:A:N6 | 53:DA:899:A:O2' | 2.32 | 0.62 |
| 27:CF:7:TYR:OH | 27:CF:172:ALA:O | 2.17 | 0.62 |
| 30:CJ:110:ALA:O | 30:CJ:114:ALA:N | 2.33 | 0.62 |
| 2:BB:133:GLU:OE2 | 2:BB:137:ARG:NH1 | 2.33 | 0.62 |
| 28:CG:159:GLY:O | 28:CG:163:ARG:NH1 | 2.33 | 0.62 |
| 4:BD:202:GLU:OE2 | 5:BE:112:ARG:NH1 | 2.33 | 0.62 |
| 22:CA:297:G:H5'' | 42:CV:85:PHE:HB2 | 1.81 | 0.61 |
| 28:CG:11:VAL:O | 28:CG:48:ASN:ND2 | 2.33 | 0.61 |
| 1:BA:465:A:H2' | 1:BA:466:A:C8 | 2.34 | 0.61 |
| 25:CD:103:ASP:O | 25:CD:105:LYS:N | 2.29 | 0.61 |
| 33:CM:93:ASN:OD1 | 33:CM:94:THR:N | 2.32 | 0.61 |
| 5:AE:79:GLY:O | 5:AE:121:HIS:N | 2.28 | 0.61 |
| 53:DA:1186:G:OP1 | 69:DA:3652:HOH:O | 2.16 | 0.61 |
| 1:AA:1225:A:H2' | 1:AA:1226:C:C5 | 2.35 | 0.61 |
| 1:AA:411:A:OP2 | 4:AD:26:ARG:NH2 | 2.33 | 0.61 |
| 24:CC:136:PRO:O | 24:CC:139:SER:OG | 2.17 | 0.61 |
| 27:CF:61:SER:O | 27:CF:63:GLN:N | 2.34 | 0.61 |
| 30:DJ:110:ALA:O | 30:DJ:114:ALA:N | 2.34 | 0.61 |
| 53:DA:456:C:OP1 | 69:DA:4875:HOH:O | 2.16 | 0.61 |
| 22:CA:2307:G:H4' | 22:CA:2308:G:O5' | 2.01 | 0.61 |
| 1:BA:531:U:H4' | 1:BA:532:A:H4' | 1.83 | 0.61 |
| 41:CU:3:ARG:HH11 | 41:CU:3:ARG:HG2 | 1.66 | 0.60 |
| 2:AB:120:GLN:O | 2:AB:125:THR:N | 2.34 | 0.60 |
| 53:DA:545:U:H2' | 53:DA:546:U:O3' | 2.01 | 0.60 |
| 10:BJ:65:TYR:HB2 | 14:BN:96:LEU:HD11 | 1.83 | 0.60 |
| 1:BA:1492:A:OP2 | 1:BA:1493:A:N6 | 2.35 | 0.60 |
| 11:BK:92:GLY:O | 11:BK:94:GLU:N | 2.32 | 0.60 |
| 1:AA:8:A:N6 | 4:AD:202:GLU:O | 2.34 | 0.60 |
| 13:AM:3:ARG:O | 13:AM:57:ARG:NH2 | 2.33 | 0.60 |
| 53:DA:1172:C:N4 | 53:DA:1173:U:O2 | 2.35 | 0.60 |
| 7:AG:90:GLU:OE2 | 7:AG:90:GLU:N | 2.34 | 0.60 |
| 53:DA:1013:C:OP2 | 69:DA:5610:HOH:O | 2.16 | 0.60 |
| 9:AI:95:ARG:O | 9:AI:98:LEU:N | 2.35 | 0.60 |
| 5:BE:111:MET:HG3 | 5:BE:140:THR:HG21 | 1.82 | 0.60 |
| 22:CA:2171:A:O2' | 22:CA:2173:A:OP1 | 2.19 | 0.60 |
| 17:AQ:60:GLU:OE1 | 17:AQ:77:ARG:NE | 2.33 | 0.60 |
| 4:BD:99:ASP:OD1 | 4:BD:100:ASN:N | 2.35 | 0.60 |
| 35:DO:114:GLU:OE2 | 35:DO:118:ARG:NH2 | 2.33 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:DA:2609:U:C6 | 66:DA:3194:EDO:H12 | 2.36 | 0.60 |
| 20:BT:67:ILE:HG13 | 20:BT:71:LYS:HD3 | 1.84 | 0.60 |
| 10:AJ:63:ASP:HB3 | 10:AJ:65:TYR:CE1 | 2.36 | 0.60 |
| 12:AL:110:ARG:NH1 | 12:AL:112:GLN:O | 2.34 | 0.60 |
| 9:AI:88:MET:SD | 9:AI:95:ARG:HG2 | 2.42 | 0.60 |
| 1:BA:846:G:OP1 | 18:BR:48:ARG:NH2 | 2.33 | 0.60 |
| 22:CA:2131:U:H5' | 22:CA:2132:U:H5'' | 1.84 | 0.60 |
| 36:CP:17:LYS:HA | 36:CP:17:LYS:HE2 | 1.84 | 0.60 |
| 1:AA:844:G:N3 | 1:AA:844:G:H2' | 2.16 | 0.60 |
| 52:C5:26:ILE:HD13 | 52:C5:26:ILE:H | 1.66 | 0.60 |
| 14:AN:31:ILE:HA | 14:AN:34:VAL:HG23 | 1.84 | 0.59 |
| 45:DY:72:ARG:O | 45:DY:75:GLY:N | 2.28 | 0.59 |
| 1:BA:537:G:OP1 | 12:BL:110:ARG:NH2 | 2.34 | 0.59 |
| 1:AA:1178:G:N2 | 1:AA:1181:G:OP2 | 2.34 | 0.59 |
| 22:CA:605:G:N3 | 22:CA:657:U:O2' | 2.34 | 0.59 |
| 15:BO:64:ARG:NH1 | 15:BO:68:ASP:OD1 | 2.35 | 0.59 |
| 25:CD:149:ASN:OD1 | 25:CD:150:GLN:N | 2.35 | 0.59 |
| 11:AK:112:ASP:HB3 | 21:AU:2:PRO:HG2 | 1.83 | 0.59 |
| 53:DA:558:U:OP2 | 69:DA:5211:HOH:O | 2.15 | 0.59 |
| 1:AA:1228:C:P | 13:AM:107:ARG:HH22 | 2.26 | 0.59 |
| 53:DA:297:G:OP2 | 69:DA:7999:HOH:O | 2.16 | 0.59 |
| 1:BA:1060:U:OP1 | 14:BN:85:ARG:NH2 | 2.36 | 0.59 |
| 1:AA:427:U:O2' | 1:AA:541:G:OP1 | 2.21 | 0.59 |
| 5:BE:45:ARG:HA | 5:BE:72:ILE:O | 2.01 | 0.59 |
| 23:CB:30:C:OP1 | 36:CP:3:LYS:NZ | 2.35 | 0.59 |
| 5:AE:161:VAL:HG12 | 5:AE:162:GLU:H | 1.67 | 0.59 |
| 16:BP:78:VAL:O | 16:BP:79:ASN:HB2 | 2.01 | 0.59 |
| 1:BA:476:U:O4 | 69:BA:1912:HOH:O | 2.17 | 0.59 |
| 53:DA:141:G:H2' | 53:DA:142:A:C2 | 2.37 | 0.59 |
| 22:CA:207:A:OP2 | 69:CA:3827:HOH:O | 2.16 | 0.59 |
| 1:BA:1492:A:H2' | 22:CA:1913:A:C6 | 2.38 | 0.59 |
| 55:DI:132:TYR:N | 55:DI:133:GLU:HB2 | 2.16 | 0.59 |
| 22:CA:1368:G:N7 | 69:CA:3533:HOH:O | 2.31 | 0.59 |
| 8:BH:3:MET:N | 8:BH:3:MET:SD | 2.75 | 0.59 |
| 22:CA:826:U:O2' | 33:CM:53:GLY:HA3 | 2.03 | 0.59 |
| 36:DP:68:LYS:HB3 | 61:DP:201:PEG:H22 | 1.84 | 0.59 |
| 5:BE:157:ARG:O | 5:BE:159:LYS:N | 2.34 | 0.59 |
| 5:BE:154:ALA:C | 5:BE:156:LYS:H | 2.07 | 0.59 |
| 53:DA:1171:G:C4 | 53:DA:1172:C:N4 | 2.71 | 0.59 |
| 1:AA:80:A:C2 | 1:AA:90:C:N3 | 2.71 | 0.59 |
| 22:CA:1534:U:O2' | 22:CA:1537:G:O6 | 2.20 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 53:DA:787:C:OP1 | 59:DA:3223:PUT:N1 | 2.36 | 0.58 |
| 53:DA:711:G:OP1 | 69:DA:5064:HOH:O | 2.16 | 0.58 |
| 53:DA:2683:C:O2 | 32:DL:70:ARG:NH2 | 2.30 | 0.58 |
| 1:BA:1493:A:OP2 | 1:BA:1493:A:C8 | 2.56 | 0.58 |
| 29:DH:41:LYS:HA | 29:DH:44:ILE:HG23 | 1.84 | 0.58 |
| 1:AA:825:A:O2' | 8:AH:13:ARG:NH1 | 2.37 | 0.58 |
| 7:BG:68:ASN:O | 7:BG:138:ARG:NH1 | 2.36 | 0.58 |
| 47:D0:10:THR:HG22 | 47:D0:11:ARG:HG3 | 1.85 | 0.58 |
| 3:BC:126:ARG:O | 3:BC:127:ARG:HB2 | 2.03 | 0.58 |
| 53:DA:1119:U:OP2 | 69:DA:5002:HOH:O | 2.16 | 0.58 |
| 22:CA:646:U:C5' | 22:CA:647:G:H5'' | 2.33 | 0.58 |
| 23:DB:23:G:O6 | 69:DB:304:HOH:O | 2.17 | 0.58 |
| 53:DA:1292:G:N3 | 69:DA:6760:HOH:O | 2.31 | 0.58 |
| 27:CF:122:PHE:O | 27:CF:124:GLY:N | 2.35 | 0.58 |
| 8:BH:64:LYS:HB3 | 8:BH:71:VAL:HG21 | 1.86 | 0.58 |
| 9:BI:88:MET:SD | 9:BI:95:ARG:HG2 | 2.44 | 0.58 |
| 19:AS:29:LYS:HB3 | 19:AS:30:PRO:HD2 | 1.85 | 0.58 |
| 13:BM:4:ILE:O | 13:BM:6:GLY:N | 2.36 | 0.58 |
| 4:AD:78:GLU:OE2 | 4:AD:81:ARG:NH2 | 2.36 | 0.58 |
| 5:BE:100:SER:O | 5:BE:122:ASN:ND2 | 2.37 | 0.58 |
| 15:BO:17:ARG:HD3 | 15:BO:17:ARG:N | 2.19 | 0.58 |
| 53:DA:2886[B]:A:N3 | 53:DA:2886[B]:A:H2' | 2.17 | 0.58 |
| 1:BA:521:G:OP1 | 69:BA:1874:HOH:O | 2.17 | 0.58 |
| 53:DA:15:G:OP2 | 69:DA:5595:HOH:O | 2.16 | 0.58 |
| 51:D4:63:PRO:O | 69:D4:128:HOH:O | 2.17 | 0.58 |
| 22:CA:666:A:H4' | 33:CM:48:ARG:HD2 | 1.86 | 0.58 |
| 22:CA:784:G:H5' | 22:CA:785:G:OP1 | 2.04 | 0.58 |
| 26:CE:41:GLN:O | 26:CE:43:THR:N | 2.30 | 0.58 |
| 5:BE:156:LYS:HD2 | 8:BH:71:VAL:HG13 | 1.85 | 0.58 |
| 53:DA:2674:G:H4' | 32:DL:30:ARG:HD2 | 1.85 | 0.58 |
| 1:BA:991:U:H4' | 1:BA:992:U:H5'' | 1.86 | 0.58 |
| 8:AH:113:ASP:OD1 | 8:AH:117:ARG:NH2 | 2.37 | 0.58 |
| 53:DA:2275:C:C6 | 57:DA:3193:PG4:H41 | 2.38 | 0.58 |
| 53:DA:2872:A:N7 | 69:DA:4918:HOH:O | 2.32 | 0.58 |
| 10:AJ:48:ARG:NH1 | 10:AJ:66:GLU:OE1 | 2.37 | 0.58 |
| 53:DA:948:C:O2' | 63:DA:3203:1PE:H241 | 2.04 | 0.57 |
| 53:DA:1171:G:H2' | 53:DA:1172:C:C4 | 2.39 | 0.57 |
| 7:BG:92:ARG:HB3 | 7:BG:93:PRO:HD2 | 1.86 | 0.57 |
| 27:DF:158:THR:HG22 | 27:DF:160:ALA:H | 1.69 | 0.57 |
| 55:DI:103:ASN:O | 55:DI:105:LYS:N | 2.37 | 0.57 |
| 37:DQ:31:TRP:CD1 | 57:DQ:202:PG4:H31 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:DA:1171:G:H2' | 53:DA:1172:C:C5 | 2.39 | 0.57 |
| 1:BA:1329:A:H5" | 13:BM:26:GLY:H | 1.69 | 0.57 |
| 1:AA:691:G:O6 | 11:AK:57:LYS:NZ | 2.33 | 0.57 |
| 53:DA:1665:A:OP1 | 69:DA:4215:HOH:O | 2.17 | 0.57 |
| 1:BA:825:A:O2' | 8:BH:13:ARG:NH1 | 2.37 | 0.57 |
| 22:CA:1779:U:H5 | 22:CA:1784:A:N7 | 2.02 | 0.57 |
| 53:DA:2831:G:OP1 | 54:DD:56:LYS:NZ | 2.36 | 0.57 |
| 53:DA:1698:A:OP2 | 59:DA:3213:PUT:H22 | 2.05 | 0.57 |
| 14:AN:21:PHE:HA | 14:AN:25:ALA:HB3 | 1.85 | 0.57 |
| 54:DD:149:ASN:OD1 | 54:DD:150[B]:MEQ:N | 2.36 | 0.57 |
| 33:CM:29:LYS:O | 33:CM:31:GLY:N | 2.37 | 0.57 |
| 22:CA:396:G:H1' | 45:CY:29:PHE:HB3 | 1.84 | 0.57 |
| 22:CA:1143:A:OP2 | 69:CA:3517:HOH:O | 2.17 | 0.57 |
| 30:CJ:100:LYS:HA | 30:CJ:139:VAL:O | 2.04 | 0.57 |
| 32:CL:107:LEU:O | 32:CL:109:SER:N | 2.37 | 0.57 |
| 22:CA:1754:A:N1 | 22:CA:2716:C:O2' | 2.35 | 0.57 |
| 13:BM:81:MET:O | 13:BM:92:ARG:NH2 | 2.37 | 0.57 |
| 53:DA:2286:G:OP2 | 49:D2:6:ARG:NH2 | 2.37 | 0.57 |
| 53:DA:136:G:C2 | 53:DA:144:A:C2 | 2.92 | 0.57 |
| 1:BA:100:G:OP2 | 69:BA:1869:HOH:O | 2.17 | 0.57 |
| 28:DG:127:THR:HG22 | 28:DG:129:THR:H | 1.70 | 0.57 |
| 35:CO:45:ARG:HG2 | 35:CO:95:THR:HG21 | 1.86 | 0.57 |
| 25:CD:151:THR:HG22 | 25:CD:152:PRO:N | 2.19 | 0.57 |
| 18:AR:37:GLY:O | 18:AR:63:ARG:NH2 | 2.35 | 0.57 |
| 1:AA:1060:U:OP1 | 14:AN:85:ARG:NH2 | 2.37 | 0.57 |
| 1:AA:207:C:N4 | 1:AA:212:G:O6 | 2.37 | 0.57 |
| 1:BA:1109:C:C2' | 1:BA:1110:A:H5" | 2.35 | 0.57 |
| 14:BN:49:GLN:NE2 | 19:BS:10:PHE:CE2 | 2.73 | 0.57 |
| 53:DA:585:G:N7 | 38:DR:6:ARG:NH1 | 2.48 | 0.57 |
| 53:DA:2441:U:O2' | 62:DA:3225:SPD:H91 | 2.04 | 0.57 |
| 53:DA:142:A:H2' | 53:DA:143:C:C6 | 2.40 | 0.57 |
| 53:DA:1172:C:C4 | 53:DA:1173:U:H1' | 2.39 | 0.57 |
| 53:DA:2257:U:O2 | 57:DA:3193:PG4:H71 | 2.04 | 0.57 |
| 53:DA:2434:A:N7 | 69:DA:6970:HOH:O | 2.32 | 0.57 |
| 22:CA:2550:G:O6 | 22:CA:2551:C:N4 | 2.38 | 0.57 |
| 12:BL:7:LEU:HD22 | 12:BL:12:ARG:HD2 | 1.87 | 0.57 |
| 14:BN:21:PHE:C | 14:BN:26:GLU:OE1 | 2.44 | 0.56 |
| 3:AC:126:ARG:O | 3:AC:127:ARG:HB2 | 2.05 | 0.56 |
| 1:BA:483:C:O2 | 16:BP:13:LYS:NZ | 2.38 | 0.56 |
| 1:BA:1317:C:H2' | 14:BN:49:GLN:HE21 | 1.70 | 0.56 |
| 53:DA:357:C:H2' | 53:DA:358:U:C6 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:DA:1020:A:C2 | 53:DA:1141:U:C2 | 2.93 | 0.56 |
| 46:CZ:7:ARG:HG2 | 46:CZ:56:LEU:HD13 | 1.87 | 0.56 |
| 10:AJ:57:VAL:HG22 | 10:AJ:58:ASN:H | 1.70 | 0.56 |
| 1:AA:261:U:OP2 | 20:AT:74:ARG:NH2 | 2.38 | 0.56 |
| 48:D1:16:ARG:O | 69:D1:208:HOH:O | 2.17 | 0.56 |
| 22:CA:2004:G:OP2 | 69:CA:3658:HOH:O | 2.18 | 0.56 |
| 53:DA:544:C:H3' | 53:DA:545:U:C2 | 2.41 | 0.56 |
| 13:BM:93:ARG:NH2 | 19:BS:80:TYR:OH | 2.39 | 0.56 |
| 53:DA:1478:G:H1 | 53:DA:1513:U:H3 | 1.54 | 0.56 |
| 36:CP:33:ARG:O | 36:CP:34:HIS:HB2 | 2.05 | 0.56 |
| 1:AA:203:G:N2 | 1:AA:204:G:O6 | 2.39 | 0.56 |
| 62:DA:3225:SPD:H82 | 69:DA:5539:HOH:O | 2.06 | 0.56 |
| 11:BK:119:ASN:OD1 | 21:BU:35:ARG:NH1 | 2.36 | 0.56 |
| 22:CA:2469:A:O2' | 34:CN:55:ARG:NH2 | 2.35 | 0.56 |
| 22:CA:192:C:O2' | 22:CA:802:A:N3 | 2.34 | 0.56 |
| 45:DY:41:GLU:N | 69:DY:102:HOH:O | 2.39 | 0.56 |
| 1:BA:840:C:C5 | 1:BA:842:U:H5' | 2.41 | 0.56 |
| 53:DA:788:A:H3' | 59:DA:3223:PUT:H41 | 1.88 | 0.56 |
| 30:CJ:100:LYS:HB2 | 30:CJ:141:GLU:HB2 | 1.88 | 0.56 |
| 42:CV:74:ASN:C | 42:CV:76:ALA:H | 2.10 | 0.56 |
| 24:CC:260:ASN:O | 24:CC:262:ARG:N | 2.39 | 0.56 |
| 3:BC:179:ARG:HD2 | 3:BC:206:GLU:HB2 | 1.88 | 0.56 |
| 26:CE:52:VAL:HG21 | 26:CE:81:GLY:CA | 2.35 | 0.56 |
| 6:BF:3:HIS:HB2 | 6:BF:92:THR:HG23 | 1.87 | 0.56 |
| 1:AA:1135:U:N3 | 1:AA:1137:C:O2 | 2.40 | 0.56 |
| 1:BA:81:A:N7 | 1:BA:83:C:N4 | 2.54 | 0.56 |
| 1:BA:1189:U:OP1 | 14:BN:98:LYS:NZ | 2.39 | 0.56 |
| 30:DJ:19:ASN:HA | 30:DJ:39:CYS:SG | 2.46 | 0.55 |
| 1:BA:404:G:N7 | 4:BD:2:ALA:HB3 | 2.21 | 0.55 |
| 24:CC:158:ALA:HB1 | 24:CC:197:ASN:HB3 | 1.87 | 0.55 |
| 39:DS:21:ARG:HH21 | 57:DS:202:PG4:H71 | 1.71 | 0.55 |
| 22:CA:526:A:OP1 | 69:CA:3842:HOH:O | 2.18 | 0.55 |
| 22:CA:614:A:O2' | 22:CA:615:U:OP2 | 2.25 | 0.55 |
| 1:BA:451:A:H2' | 69:BA:1918:HOH:O | 2.06 | 0.55 |
| 9:AI:84:THR:HG21 | 9:AI:103:PHE:HB3 | 1.87 | 0.55 |
| 18:BR:42:SER:O | 18:BR:46:GLY:N | 2.40 | 0.55 |
| 36:CP:52:SER:OG | 36:CP:53:THR:N | 2.39 | 0.55 |
| 30:DJ:100:LYS:HA | 30:DJ:139:VAL:O | 2.06 | 0.55 |
| 8:BH:88:ARG:O | 8:BH:89:LYS:HB3 | 2.06 | 0.55 |
| 5:BE:26:LYS:HE3 | 5:BE:26:LYS:HA | 1.87 | 0.55 |
| 10:AJ:7:ARG:HG2 | 10:AJ:101:SER:HB2 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:CZ:11:VAL:O | 46:CZ:15:ASN:ND2 | 2.39 | 0.55 |
| 7:BG:90:GLU:OE1 | 7:BG:90:GLU:N | 2.40 | 0.55 |
| 54:DD:149:ASN:OD1 | 54:DD:150[A]:MEQ:N | 2.36 | 0.55 |
| 22:CA:370:G:N7 | 69:CA:3474:HOH:O | 2.33 | 0.55 |
| 23:DB:2:G:C2 | 23:DB:119:A:C2 | 2.95 | 0.55 |
| 38:CR:9:ILE:HD12 | 38:CR:9:ILE:C | 2.27 | 0.55 |
| 7:BG:37:SER:O | 7:BG:41:SER:OG | 2.24 | 0.55 |
| 22:CA:2359:C:O2 | 33:CM:60:ARG:NH2 | 2.39 | 0.55 |
| 1:BA:1366:C:O2' | 10:BJ:62:ARG:NH2 | 2.38 | 0.55 |
| 22:CA:1993:U:H4' | 25:CD:133:THR:HG22 | 1.88 | 0.55 |
| 53:DA:1847:A:H8 | 53:DA:1847:A:P | 2.30 | 0.55 |
| 35:CO:56:LYS:NZ | 35:CO:87:PHE:O | 2.39 | 0.55 |
| 1:BA:394:G:OP2 | 69:BA:1887:HOH:O | 2.18 | 0.55 |
| 48:D1:12:LYS:NZ | 69:D1:240:HOH:O | 2.38 | 0.55 |
| 6:AF:16:GLU:HG2 | 4:BD:193:ALA:HA | 1.87 | 0.55 |
| 1:AA:976:G:OP2 | 1:AA:1358:U:O2' | 2.25 | 0.55 |
| 32:CL:70:ARG:NH1 | 32:CL:74:GLY:O | 2.40 | 0.55 |
| 33:CM:111:ILE:HG22 | 33:CM:112:LEU:N | 2.21 | 0.55 |
| 1:AA:842:U:H3' | 1:AA:843:U:C5' | 2.37 | 0.55 |
| 1:BA:6:G:O6 | 5:BE:100:SER:N | 2.22 | 0.55 |
| 28:CG:70:ALA:O | 28:CG:74:SER:OG | 2.25 | 0.55 |
| 53:DA:2031:A:C6 | 53:DA:2498:OMC:H1' | 2.42 | 0.55 |
| 53:DA:282:A:H2' | 53:DA:283:G:C8 | 2.42 | 0.55 |
| 22:CA:2507:C:OP1 | 69:CA:3600:HOH:O | 2.18 | 0.55 |
| 32:DL:107:LEU:O | 32:DL:109:SER:N | 2.40 | 0.55 |
| 22:CA:1170:C:H2' | 22:CA:1171:G:H8 | 1.72 | 0.55 |
| 53:DA:1171:G:N3 | 53:DA:1179:G:N2 | 2.56 | 0.54 |
| 53:DA:189:G:N7 | 66:DA:3197:EDO:H21 | 2.22 | 0.54 |
| 7:BG:16:PRO:HB3 | 9:BI:43:THR:HG23 | 1.88 | 0.54 |
| 22:CA:1394:U:H4' | 22:CA:1603:A:H4' | 1.89 | 0.54 |
| 22:CA:301:G:OP2 | 42:CV:82:ARG:NH1 | 2.40 | 0.54 |
| 13:AM:6:GLY:CA | 13:AM:66:GLU:HG3 | 2.37 | 0.54 |
| 1:AA:1226:C:N4 | 13:AM:103:LYS:HE3 | 2.22 | 0.54 |
| 22:CA:2360:G:H1' | 33:CM:60:ARG:HD3 | 1.88 | 0.54 |
| 33:DM:85:VAL:HB | 33:DM:94:THR:CG2 | 2.37 | 0.54 |
| 22:CA:1941:C:OP2 | 69:CA:3788:HOH:O | 2.18 | 0.54 |
| 1:AA:1217:C:P | 14:AN:9:ARG:HH21 | 2.29 | 0.54 |
| 22:CA:2334:U:O4 | 36:CP:16:ARG:NH2 | 2.40 | 0.54 |
| 2:AB:27:MET:HE1 | 2:AB:187:VAL:HG12 | 1.88 | 0.54 |
| 7:BG:113:ASP:OD2 | 7:BG:122:ASN:ND2 | 2.40 | 0.54 |
| 26:CE:98:LYS:NZ | 69:CE:303:HOH:O | 2.40 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 50:C3:44:VAL:HG13 | 50:C3:45:SER:H | 1.72 | 0.54 |
| 29:CH:79:THR:HA | 29:CH:145:ASN:HB2 | 1.88 | 0.54 |
| 53:DA:142:A:C5 | 53:DA:143:C:C4 | 2.95 | 0.54 |
| 14:BN:53:ARG:HH22 | 19:BS:37:ARG:NH2 | 2.06 | 0.54 |
| 22:CA:550:C:H2' | 22:CA:551:G:H5'' | 1.90 | 0.54 |
| 55:DI:22:ALA:HA | 55:DI:86:THR:HA | 1.88 | 0.54 |
| 22:CA:585:G:N7 | 38:CR:6:ARG:NH1 | 2.50 | 0.54 |
| 1:BA:1134:G:N2 | 1:BA:1140:C:N3 | 2.56 | 0.54 |
| 53:DA:953:G:OP2 | 34:DN:18[B]:ARG:NH1 | 2.41 | 0.54 |
| 3:AC:7:PRO:HG2 | 3:AC:184:TYR:CG | 2.42 | 0.54 |
| 41:CU:69:ARG:NH1 | 41:CU:69:ARG:HB3 | 2.23 | 0.54 |
| 40:CT:84:ARG:HB2 | 40:CT:96:ILE:HG12 | 1.88 | 0.54 |
| 22:CA:430:A:N7 | 69:CA:3729:HOH:O | 2.34 | 0.54 |
| 53:DA:2297:A:H5'' | 53:DA:2297:A:C8 | 2.42 | 0.54 |
| 22:CA:139:U:O2' | 22:CA:141:G:N1 | 2.36 | 0.54 |
| 42:DV:45:HIS:CD2 | 42:DV:58:ILE:HD13 | 2.43 | 0.54 |
| 10:AJ:40:ILE:CG1 | 10:AJ:73:LEU:HB3 | 2.37 | 0.54 |
| 8:BH:106:THR:HG21 | 8:BH:121:LEU:HD13 | 1.89 | 0.54 |
| 55:DI:131:THR:OG1 | 55:DI:133:GLU:O | 2.19 | 0.54 |
| 27:DF:119:ALA:O | 27:DF:167:ARG:NH1 | 2.41 | 0.54 |
| 1:AA:1189:U:OP1 | 14:AN:98:LYS:NZ | 2.38 | 0.54 |
| 1:AA:407:U:OP1 | 4:AD:3:ARG:NH2 | 2.40 | 0.54 |
| 22:CA:2189:U:H2' | 22:CA:2190:G:H5' | 1.90 | 0.54 |
| 15:BO:89:ARG:NH1 | 22:CA:716:A:OP1 | 2.41 | 0.54 |
| 50:D3:29:GLN:HG2 | 61:D3:102:PEG:H21 | 1.91 | 0.54 |
| 36:DP:68:LYS:HE3 | 61:DP:201:PEG:H41 | 1.89 | 0.54 |
| 53:DA:550:C:H2' | 53:DA:551:G:H5'' | 1.89 | 0.54 |
| 23:CB:90:C:H6 | 23:CB:90:C:H5'' | 1.72 | 0.54 |
| 1:BA:1217:C:OP2 | 14:BN:9:ARG:NH2 | 2.33 | 0.54 |
| 11:AK:16:VAL:HG23 | 11:AK:17:SER:H | 1.72 | 0.54 |
| 10:AJ:65:TYR:HB3 | 14:AN:96:LEU:HD11 | 1.90 | 0.53 |
| 53:DA:551:G:H8 | 53:DA:551:G:H5' | 1.73 | 0.53 |
| 22:CA:1170:C:H2' | 22:CA:1171:G:C8 | 2.42 | 0.53 |
| 1:BA:1144:G:N2 | 1:BA:1145:A:C2 | 2.76 | 0.53 |
| 12:BL:65:SER:HB2 | 12:BL:82:ILE:HD11 | 1.89 | 0.53 |
| 53:DA:2172:U:H4' | 53:DA:2173:A:H5' | 1.90 | 0.53 |
| 22:CA:582:A:N7 | 69:CA:3262:HOH:O | 2.34 | 0.53 |
| 34:DN:89:VAL:CG1 | 58:DN:201:MPD:HM3 | 2.38 | 0.53 |
| 13:AM:79:ARG:NH1 | 27:DF:113:ASP:OD1 | 2.41 | 0.53 |
| 22:CA:184:C:O2' | 22:CA:217:A:N3 | 2.35 | 0.53 |
| 1:AA:951:G:OP2 | 13:AM:101:ARG:NH2 | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:BA:196:A:OP1 | 20:BT:64:LYS:NZ | 2.40 | 0.53 |
| 9:AI:85:ARG:HA | 9:AI:88:MET:HE3 | 1.90 | 0.53 |
| 22:CA:1993:U:H4' | 25:CD:133:THR:CG2 | 2.38 | 0.53 |
| 1:AA:843:U:OP1 | 1:AA:846:G:N2 | 2.42 | 0.53 |
| 23:CB:35:C:C2' | 23:CB:36:C:H5' | 2.38 | 0.53 |
| 11:BK:83:GLU:OE2 | 11:BK:109:ASN:ND2 | 2.41 | 0.53 |
| 13:AM:8:ASN:OD1 | 13:AM:9:ILE:N | 2.42 | 0.53 |
| 1:AA:769:G:H4' | 1:AA:1513:A:H4' | 1.90 | 0.53 |
| 48:C1:55:ILE:HG22 | 48:C1:56:ALA:N | 2.23 | 0.53 |
| 53:DA:2383:G:O6 | 69:DA:4990:HOH:O | 2.18 | 0.53 |
| 22:CA:2127:G:N2 | 22:CA:2161:C:O2 | 2.40 | 0.53 |
| 1:BA:72:A:C6 | 1:BA:73:C:N3 | 2.76 | 0.53 |
| 1:AA:617:G:O2' | 69:AA:1936:HOH:O | 2.18 | 0.53 |
| 6:BF:50:PRO:CD | 18:BR:74:HIS:HB3 | 2.39 | 0.53 |
| 1:BA:35:G:N3 | 12:BL:115:SER:OG | 2.42 | 0.53 |
| 17:BQ:60:GLU:OE2 | 17:BQ:77:ARG:NH1 | 2.42 | 0.53 |
| 53:DA:142:A:O2' | 53:DA:143:C:O4' | 2.25 | 0.53 |
| 1:BA:374:A:H5'' | 1:BA:452:A:N1 | 2.23 | 0.53 |
| 27:DF:112:ARG:NH1 | 27:DF:134:GLU:OE2 | 2.41 | 0.53 |
| 22:CA:528:A:C2 | 22:CA:2042:A:H2' | 2.43 | 0.53 |
| 10:AJ:40:ILE:HG12 | 10:AJ:73:LEU:HB3 | 1.89 | 0.53 |
| 1:BA:774:G:H21 | 57:BA:1642:PG4:H52 | 1.74 | 0.53 |
| 22:CA:1419:A:O2' | 22:CA:1421:G:N7 | 2.32 | 0.53 |
| 1:AA:404:G:N7 | 4:AD:2:ALA:HB3 | 2.23 | 0.53 |
| 14:BN:25:ALA:HA | 14:BN:28:LYS:HG2 | 1.90 | 0.53 |
| 5:AE:149:SER:HB3 | 5:AE:152:MET:CG | 2.39 | 0.53 |
| 14:BN:28:LYS:O | 14:BN:31:ILE:HG22 | 2.09 | 0.53 |
| 19:BS:10:PHE:CD2 | 19:BS:11:ILE:N | 2.77 | 0.53 |
| 53:DA:45:G:H5'' | 53:DA:46:G:H5' | 1.89 | 0.53 |
| 1:AA:526:C:C2' | 1:AA:527:G7M:H5' | 2.39 | 0.53 |
| 26:CE:152:GLU:O | 26:CE:154:ASP:N | 2.42 | 0.53 |
| 29:DH:68:ARG:NH2 | 29:DH:114:GLU:OE1 | 2.42 | 0.53 |
| 49:C2:25:LYS:NZ | 49:C2:32:GLU:O | 2.36 | 0.53 |
| 1:AA:1379:G:N7 | 7:AG:2:PRO:HB2 | 2.24 | 0.53 |
| 22:CA:45:G:H5'' | 22:CA:46:G:H5' | 1.92 | 0.52 |
| 53:DA:1046:A:H4' | 55:DI:58:THR:HG21 | 1.91 | 0.52 |
| 38:DR:58:ARG:HA | 38:DR:61:TRP:CE3 | 2.44 | 0.52 |
| 46:CZ:7:ARG:O | 46:CZ:60:LYS:NZ | 2.42 | 0.52 |
| 2:BB:126:PHE:C | 2:BB:128:LYS:H | 2.10 | 0.52 |
| 53:DA:550:C:C2' | 53:DA:551:G:H5'' | 2.39 | 0.52 |
| 20:BT:44:LYS:HD3 | 20:BT:87:ALA:HA | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 15:AO:20:ASN:O | 15:AO:22:THR:N | 2.41 | 0.52 |
| 1:AA:1124:G:H5' | 10:AJ:37:ARG:HH11 | 1.73 | 0.52 |
| 7:BG:109:ARG:O | 7:BG:119:ARG:NH2 | 2.42 | 0.52 |
| 22:CA:2526:G:O2' | 52:C5:1:MET:HB3 | 2.09 | 0.52 |
| 1:AA:938:A:H5' | 7:AG:76:LYS:NZ | 2.23 | 0.52 |
| 1:BA:264:C:O2' | 17:BQ:66:PRO:O | 2.26 | 0.52 |
| 7:BG:130:ASN:HA | 7:BG:135:VAL:HG11 | 1.91 | 0.52 |
| 53:DA:141:G:H3' | 53:DA:142:A:C5 | 2.44 | 0.52 |
| 30:CJ:100:LYS:HB3 | 30:CJ:141:GLU:HB2 | 1.89 | 0.52 |
| 53:DA:1170:C:H2' | 53:DA:1171:G:C8 | 2.44 | 0.52 |
| 34:DN:89:VAL:HG12 | 58:DN:201:MPD:HM3 | 1.90 | 0.52 |
| 22:CA:1808:A:O2' | 45:CY:3:ARG:NH1 | 2.42 | 0.52 |
| 1:BA:216:U:H5'' | 1:BA:464:U:H4' | 1.91 | 0.52 |
| 1:AA:1032:G:H2' | 1:AA:1033:G:H4' | 1.90 | 0.52 |
| 53:DA:543:G:H5'' | 53:DA:543:G:H8 | 1.74 | 0.52 |
| 1:BA:87:C:H2' | 1:BA:88:U:C6 | 2.43 | 0.52 |
| 22:CA:1869:G:H3' | 22:CA:1870:C:H5' | 1.92 | 0.52 |
| 11:BK:112:ASP:HB3 | 21:BU:2:PRO:HG2 | 1.90 | 0.52 |
| 41:CU:60:THR:O | 69:CU:102:HOH:O | 2.19 | 0.52 |
| 6:BF:51:ILE:C | 6:BF:53:LYS:H | 2.12 | 0.52 |
| 22:CA:797:G:N7 | 69:CA:3296:HOH:O | 2.34 | 0.52 |
| 52:C5:22:VAL:HG11 | 52:C5:36:ARG:HG3 | 1.90 | 0.52 |
| 53:DA:1536:C:H4' | 53:DA:1537:G:H5'' | 1.91 | 0.52 |
| 33:CM:29:LYS:O | 33:CM:30:THR:OG1 | 2.25 | 0.52 |
| 1:AA:418:C:N4 | 69:AA:1753:HOH:O | 2.43 | 0.52 |
| 41:CU:49:LYS:HD3 | 41:CU:49:LYS:N | 2.24 | 0.52 |
| 22:CA:1789:A:OP2 | 24:CC:221:ARG:NH1 | 2.41 | 0.52 |
| 13:AM:12:HIS:HA | 13:AM:45:ILE:CG1 | 2.39 | 0.52 |
| 53:DA:1105:U:H2' | 53:DA:1106:G:H8 | 1.75 | 0.52 |
| 5:BE:101:GLU:O | 5:BE:102:GLY:C | 2.48 | 0.52 |
| 1:AA:537:G:OP1 | 12:AL:110:ARG:NH2 | 2.43 | 0.52 |
| 22:CA:1011:G:OP2 | 38:CR:70:ARG:NH1 | 2.42 | 0.52 |
| 7:BG:83:SER:HB3 | 7:BG:85:TYR:CZ | 2.45 | 0.52 |
| 7:BG:15:ASP:HB2 | 7:BG:20:SER:H | 1.75 | 0.52 |
| 53:DA:2256:G:N2 | 57:DA:3193:PG4:H61 | 2.25 | 0.52 |
| 7:BG:88:PRO:HD2 | 7:BG:152:ALA:HA | 1.91 | 0.52 |
| 22:CA:842:U:O4 | 69:CA:3496:HOH:O | 2.18 | 0.52 |
| 63:DA:3185:1PE:H222 | 69:DA:6271:HOH:O | 2.09 | 0.52 |
| 53:DA:1869:G:C2 | 53:DA:1873:G:C6 | 2.98 | 0.52 |
| 31:DK:96:ARG:NH2 | 69:DK:319:HOH:O | 2.24 | 0.52 |
| 9:AI:85:ARG:HA | 9:AI:88:MET:CE | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 53:DA:2256:G:H21 | 57:DA:3193:PG4:H31 | 1.75 | 0.52 |
| 58:DN:201:MPD:O4 | 58:DN:201:MPD:HM2 | 2.08 | 0.52 |
| 1:BA:374:A:H5'' | 1:BA:452:A:C2 | 2.44 | 0.52 |
| 11:BK:88:GLY:H | 11:BK:114:THR:HG22 | 1.74 | 0.52 |
| 13:AM:12:HIS:ND1 | 13:AM:45:ILE:HG13 | 2.24 | 0.52 |
| 10:BJ:57:VAL:HG22 | 10:BJ:58:ASN:H | 1.74 | 0.52 |
| 22:CA:388:G:N7 | 22:CA:390:U:H2' | 2.25 | 0.52 |
| 7:BG:59:LEU:H | 7:BG:59:LEU:HD23 | 1.75 | 0.52 |
| 3:BC:40:ARG:HG2 | 3:BC:55:ILE:HG12 | 1.90 | 0.52 |
| 5:BE:114:VAL:HG22 | 5:BE:115:LEU:HD13 | 1.92 | 0.52 |
| 39:DS:82:HIS:NE2 | 69:DS:341:HOH:O | 2.33 | 0.52 |
| 53:DA:1433:A:O2' | 53:DA:1434:A:H5' | 2.10 | 0.52 |
| 5:BE:154:ALA:O | 5:BE:157:ARG:N | 2.43 | 0.52 |
| 22:CA:139:U:HO2' | 22:CA:141:G:H1 | 1.55 | 0.52 |
| 53:DA:278:A:C2 | 53:DA:362:A:C8 | 2.98 | 0.52 |
| 35:CO:2:ARG:O | 35:CO:2:ARG:HD3 | 2.10 | 0.52 |
| 15:AO:26:GLU:N | 15:AO:26:GLU:OE1 | 2.35 | 0.52 |
| 1:AA:1428:A:H2' | 1:AA:1429:A:O4' | 2.10 | 0.52 |
| 32:CL:121:GLU:HG2 | 32:CL:122:VAL:HG23 | 1.91 | 0.52 |
| 1:BA:79:G:H2' | 1:BA:80:A:O4' | 2.10 | 0.52 |
| 24:CC:252:THR:HG22 | 24:CC:253:LYS:H | 1.73 | 0.52 |
| 22:CA:1915:3TD:H2' | 22:CA:1916:A:O4' | 2.10 | 0.52 |
| 50:D3:32:ALA:HB2 | 61:D3:102:PEG:H12 | 1.91 | 0.52 |
| 1:AA:412:A:H1' | 1:AA:413:G:C5' | 2.39 | 0.52 |
| 1:AA:1060:U:H4' | 10:AJ:53:ILE:HG23 | 1.91 | 0.52 |
| 53:DA:62:U:O4' | 58:DA:3205:MPD:H31 | 2.10 | 0.52 |
| 42:CV:61:LYS:HA | 42:CV:61:LYS:HE3 | 1.92 | 0.52 |
| 17:BQ:14:SER:HB3 | 17:BQ:22:VAL:HG13 | 1.92 | 0.52 |
| 31:CK:99:ARG:NH1 | 31:CK:102:GLU:OE1 | 2.43 | 0.52 |
| 22:CA:1582:C:N4 | 22:CA:1583:A:C6 | 2.78 | 0.52 |
| 5:BE:104:GLY:HA3 | 5:BE:122:ASN:CA | 2.40 | 0.51 |
| 14:BN:18:ASP:OD1 | 14:BN:19:LYS:N | 2.43 | 0.51 |
| 1:BA:1309:G:OP2 | 13:BM:98:ARG:NE | 2.39 | 0.51 |
| 22:CA:2061:G:H5'' | 22:CA:2503:2MA:HM22 | 1.92 | 0.51 |
| 8:AH:48:ASP:OD1 | 8:AH:49:PHE:N | 2.38 | 0.51 |
| 27:CF:108:VAL:HG11 | 27:CF:176:PRO:HG2 | 1.92 | 0.51 |
| 27:CF:108:VAL:HG13 | 27:CF:111:ILE:HD12 | 1.92 | 0.51 |
| 41:DU:33:LYS:HG3 | 41:DU:80:TRP:CE3 | 2.45 | 0.51 |
| 53:DA:614:A:O2' | 53:DA:615:U:OP2 | 2.26 | 0.51 |
| 1:BA:531:U:H4' | 1:BA:532:A:C5' | 2.40 | 0.51 |
| 2:AB:126:PHE:C | 2:AB:128:LYS:H | 2.13 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 53:DA:1418:G:H2' | 53:DA:1579:A:N6 | 2.26 | 0.51 |
| 14:AN:42:TRP:HD1 | 14:AN:44:ALA:N | 2.09 | 0.51 |
| 22:CA:1847:A:HO2' | 22:CA:1848:A:H8 | 1.55 | 0.51 |
| 3:BC:72:ARG:HB3 | 3:BC:75:ILE:CG2 | 2.40 | 0.51 |
| 3:BC:80:LYS:HA | 3:BC:80:LYS:HE3 | 1.92 | 0.51 |
| 53:DA:2324:U:H3' | 53:DA:2325:G:C5' | 2.40 | 0.51 |
| 22:CA:2081:U:OP1 | 45:CY:17:ASN:ND2 | 2.41 | 0.51 |
| 53:DA:2603:G:OP2 | 69:DA:4829:HOH:O | 2.19 | 0.51 |
| 24:CC:111:LYS:NZ | 24:CC:114:ASP:OD1 | 2.41 | 0.51 |
| 1:AA:181:A:N6 | 1:AA:195:A:OP2 | 2.43 | 0.51 |
| 1:AA:157:U:C2' | 1:AA:158:G:H5' | 2.40 | 0.51 |
| 22:CA:1900:A:O2' | 69:CA:3824:HOH:O | 2.19 | 0.51 |
| 22:CA:1367:A:OP1 | 69:CA:3534:HOH:O | 2.19 | 0.51 |
| 1:BA:1226:C:N4 | 13:BM:103:LYS:HE3 | 2.25 | 0.51 |
| 1:BA:1406:U:H2' | 1:BA:1407:5MC:H5' | 1.91 | 0.51 |
| 3:BC:117:ALA:HB2 | 3:BC:200:VAL:CG1 | 2.40 | 0.51 |
| 22:CA:2550:G:C6 | 22:CA:2551:C:C4 | 2.97 | 0.51 |
| 41:DU:80:TRP:HB3 | 64:DU:101:PGE:H32 | 1.92 | 0.51 |
| 53:DA:2251:OMG:OP1 | 34:DN:81[A]:4D4:NH2 | 2.34 | 0.51 |
| 5:BE:93:ARG:HG3 | 5:BE:128:TYR:HB2 | 1.93 | 0.51 |
| 22:CA:2611:C:OP2 | 69:CA:3871:HOH:O | 2.19 | 0.51 |
| 57:DA:3193:PG4:H12 | 69:DA:6907:HOH:O | 2.10 | 0.51 |
| 22:CA:1792:G:H5' | 24:CC:204:VAL:HG23 | 1.93 | 0.51 |
| 1:AA:216:U:H2' | 1:AA:217:C:C6 | 2.46 | 0.51 |
| 3:BC:42:TYR:CZ | 3:BC:90:VAL:HG21 | 2.46 | 0.51 |
| 22:CA:381:G:OP1 | 45:CY:18:ARG:NH2 | 2.37 | 0.51 |
| 1:AA:741:G:OP1 | 15:AO:35:GLN:NE2 | 2.43 | 0.51 |
| 1:BA:467:U:H3' | 1:BA:468:A:H5'' | 1.93 | 0.51 |
| 58:DA:3211:MPD:O4 | 58:DA:3211:MPD:O2 | 2.28 | 0.51 |
| 24:CC:210:ALA:HA | 24:CC:213:TRP:CE2 | 2.45 | 0.51 |
| 22:CA:2264:C:N4 | 44:CX:15:ASP:OD2 | 2.43 | 0.51 |
| 1:BA:31:G:O2' | 1:BA:48:C:N4 | 2.43 | 0.51 |
| 53:DA:789:A:OP1 | 59:DA:3223:PUT:H11 | 2.10 | 0.51 |
| 48:C1:53:LYS:HE3 | 48:C1:56:ALA:HA | 1.93 | 0.51 |
| 13:AM:12:HIS:HA | 13:AM:45:ILE:HG12 | 1.93 | 0.51 |
| 7:AG:88:PRO:HG2 | 7:AG:152:ALA:HB2 | 1.93 | 0.51 |
| 1:AA:121:U:H5'' | 1:AA:122:G:OP2 | 2.11 | 0.51 |
| 53:DA:287:G:H1 | 53:DA:353:C:H42 | 1.58 | 0.51 |
| 45:CY:10:LYS:HE3 | 45:CY:54:LYS:HD3 | 1.93 | 0.51 |
| 22:CA:2306:C:N4 | 27:CF:39:GLY:O | 2.44 | 0.51 |
| 1:AA:1449:C:C2' | 1:AA:1450:U:H5' | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:DA:784:G:H5' | 53:DA:785:G:OP1 | 2.10 | 0.51 |
| 10:AJ:15:HIS:CE1 | 10:AJ:16:ARG:HD3 | 2.46 | 0.51 |
| 1:AA:1016:A:N3 | 1:AA:1016:A:H2' | 2.26 | 0.51 |
| 6:AF:38:ARG:HB3 | 6:AF:63:ASN:HB2 | 1.92 | 0.51 |
| 42:CV:18:ASP:O | 42:CV:20:GLY:N | 2.44 | 0.51 |
| 47:C0:5:ILE:HG13 | 47:C0:6:LYS:N | 2.25 | 0.51 |
| 5:BE:133:PRO:O | 5:BE:137:VAL:HG12 | 2.10 | 0.51 |
| 22:CA:1172:C:H2' | 22:CA:1173:U:O4' | 2.10 | 0.51 |
| 27:DF:102:ARG:NH1 | 69:DF:206:HOH:O | 2.43 | 0.51 |
| 1:AA:411:A:P | 4:AD:26:ARG:HH22 | 2.33 | 0.51 |
| 1:BA:966:2MG:H2' | 1:BA:967:5MC:C6 | 2.45 | 0.51 |
| 24:DC:78:VAL:HG21 | 24:DC:110:LEU:HD21 | 1.93 | 0.51 |
| 22:CA:2286:G:H4' | 22:CA:2287:A:O5' | 2.11 | 0.51 |
| 1:AA:1299:A:H2' | 1:AA:1299:A:N3 | 2.26 | 0.51 |
| 53:DA:1171:G:C2 | 53:DA:1179:G:C2 | 2.99 | 0.51 |
| 14:AN:27:LEU:O | 14:AN:31:ILE:HG12 | 2.11 | 0.51 |
| 19:AS:29:LYS:HB3 | 19:AS:30:PRO:CD | 2.41 | 0.51 |
| 48:C1:55:ILE:HG22 | 48:C1:56:ALA:H | 1.75 | 0.51 |
| 3:BC:55:ILE:CD1 | 3:BC:66:VAL:HG13 | 2.41 | 0.51 |
| 10:AJ:6:ILE:HG13 | 10:AJ:76:ILE:HB | 1.91 | 0.51 |
| 35:CO:90:ARG:CZ | 35:CO:116:VAL:HG11 | 2.41 | 0.51 |
| 23:DB:35:C:H2' | 23:DB:36:C:H5' | 1.92 | 0.51 |
| 1:AA:722:G:N3 | 1:AA:722:G:H3' | 2.25 | 0.51 |
| 15:BO:45:GLU:HG2 | 15:BO:46:HIS:H | 1.75 | 0.51 |
| 16:AP:56:ARG:NH1 | 69:AP:102:HOH:O | 2.43 | 0.51 |
| 2:AB:117:LEU:HA | 2:AB:120:GLN:HG2 | 1.93 | 0.50 |
| 26:CE:81:GLY:N | 69:CE:301:HOH:O | 2.44 | 0.50 |
| 22:CA:138:U:OP2 | 22:CA:139:U:H5' | 2.10 | 0.50 |
| 24:CC:235:GLY:HA3 | 24:CC:239:ASN:HB2 | 1.92 | 0.50 |
| 26:CE:41:GLN:C | 26:CE:43:THR:H | 2.15 | 0.50 |
| 6:BF:50:PRO:HD3 | 18:BR:74:HIS:HB3 | 1.93 | 0.50 |
| 1:BA:202:G:HO2' | 1:BA:468:A:H8 | 1.59 | 0.50 |
| 1:BA:1406:U:C2' | 1:BA:1407:5MC:H5' | 2.42 | 0.50 |
| 2:BB:9:MET:CE | 2:BB:50:PHE:HD2 | 2.24 | 0.50 |
| 5:BE:105:ILE:HG23 | 5:BE:105:ILE:O | 2.11 | 0.50 |
| 1:BA:257:G:O6 | 69:BA:1714:HOH:O | 2.19 | 0.50 |
| 22:CA:2496:C:OP2 | 34:CN:81:4D4:H8 | 2.10 | 0.50 |
| 22:CA:579:G:O2' | 22:CA:2019:A:OP1 | 2.29 | 0.50 |
| 39:CS:49:ILE:HG22 | 39:CS:53:PHE:C | 2.31 | 0.50 |
| 22:CA:646:U:H5' | 22:CA:647:G:H5'' | 1.92 | 0.50 |
| 16:AP:46:LYS:NZ | 69:AP:101:HOH:O | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 53:DA:1913:A:H4' | 53:DA:1913:A:OP1 | 2.12 | 0.50 |
| 32:CL:1:MET:HB2 | 32:CL:67:LYS:HG3 | 1.93 | 0.50 |
| 4:BD:201:VAL:HG11 | 5:BE:103:THR:HB | 1.92 | 0.50 |
| 53:DA:2116:G:N7 | 53:DA:2165:C:N4 | 2.57 | 0.50 |
| 4:AD:99:ASP:OD1 | 4:AD:100:ASN:N | 2.45 | 0.50 |
| 53:DA:1059:G:H4' | 30:DJ:117:MET:HE2 | 1.93 | 0.50 |
| 1:BA:991:U:H4' | 1:BA:992:U:C5' | 2.41 | 0.50 |
| 24:CC:17:VAL:HB | 24:CC:204:VAL:HG13 | 1.93 | 0.50 |
| 22:CA:981:A:OP2 | 22:CA:982:C:N4 | 2.40 | 0.50 |
| 15:BO:67:LEU:HD22 | 15:BO:88:ARG:HH22 | 1.77 | 0.50 |
| 1:BA:1462:C:O2' | 37:CQ:111:LYS:NZ | 2.44 | 0.50 |
| 54:DD:18:ASP:HB2 | 57:DQ:202:PG4:H82 | 1.93 | 0.50 |
| 1:AA:841:C:C5 | 1:AA:843:U:H5' | 2.47 | 0.50 |
| 53:DA:1090:A:N1 | 53:DA:1101:U:O2 | 2.45 | 0.50 |
| 8:AH:18:GLN:CG | 8:AH:70:ALA:HB1 | 2.42 | 0.50 |
| 10:BJ:81:GLU:HA | 10:BJ:84:VAL:HG12 | 1.92 | 0.50 |
| 22:CA:1665:A:H5'' | 32:CL:66:LYS:HG2 | 1.92 | 0.50 |
| 7:BG:57:SER:OG | 7:BG:58:GLU:N | 2.44 | 0.50 |
| 13:AM:16:VAL:HG12 | 13:AM:17:ILE:HD12 | 1.93 | 0.50 |
| 20:BT:27:MET:HG3 | 20:BT:28:MET:N | 2.27 | 0.50 |
| 13:BM:10:PRO:HB2 | 13:BM:18:ALA:HB1 | 1.94 | 0.50 |
| 66:DA:3210:EDO:H21 | 38:DR:16:LYS:HG3 | 1.94 | 0.50 |
| 1:BA:1183:U:O2' | 1:BA:1184:G:O5' | 2.30 | 0.50 |
| 53:DA:2887[B]:A:H2' | 53:DA:2888[B]:C:O4' | 2.11 | 0.50 |
| 53:DA:2325:G:C6 | 53:DA:2326:C:N4 | 2.79 | 0.50 |
| 29:DH:7:ASP:OD1 | 29:DH:8:LYS:N | 2.44 | 0.50 |
| 2:AB:130:THR:O | 2:AB:131:LYS:HB2 | 2.10 | 0.50 |
| 22:CA:1390:U:H2' | 22:CA:1391:U:H5' | 1.94 | 0.50 |
| 38:CR:22:LYS:HE2 | 38:CR:22:LYS:HA | 1.93 | 0.50 |
| 22:CA:971:G:OP2 | 22:CA:974:G:N2 | 2.44 | 0.50 |
| 7:BG:51:ALA:O | 7:BG:55:GLY:N | 2.36 | 0.50 |
| 31:DK:23:LYS:HE2 | 31:DK:142:ILE:OXT | 2.12 | 0.50 |
| 30:CJ:19:ASN:N | 30:CJ:20:PRO:HD2 | 2.26 | 0.50 |
| 30:DJ:100:LYS:HB3 | 30:DJ:141:GLU:HB2 | 1.93 | 0.50 |
| 53:DA:1172:C:C5 | 53:DA:1173:U:N1 | 2.80 | 0.50 |
| 1:AA:204:G:C3' | 1:AA:205:A:H5'' | 2.42 | 0.50 |
| 38:CR:9:ILE:HD12 | 38:CR:10:ALA:N | 2.27 | 0.50 |
| 6:BF:52:ASN:O | 6:BF:53:LYS:HB2 | 2.12 | 0.50 |
| 1:BA:276:G:OP1 | 17:BQ:14:SER:OG | 2.21 | 0.50 |
| 22:CA:662:G:O3' | 33:CM:16:GLY:HA2 | 2.11 | 0.50 |
| 50:D3:12:ARG:HH21 | 50:D3:12:ARG:HG2 | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:BA:147:G:N2 | 1:BA:175:C:O2 | 2.45 | 0.50 |
| 2:BB:130:THR:O | 2:BB:131:LYS:HB2 | 2.11 | 0.50 |
| 25:CD:112:THR:O | 25:CD:195:GLY:HA2 | 2.12 | 0.50 |
| 22:CA:1422:G:N2 | 22:CA:1577:C:H1' | 2.27 | 0.50 |
| 33:DM:79:LEU:HD11 | 33:DM:112:LEU:HD12 | 1.94 | 0.50 |
| 53:DA:1758:U:OP2 | 69:DA:4561:HOH:O | 2.19 | 0.50 |
| 53:DA:664:G:OP2 | 69:DA:5108:HOH:O | 2.19 | 0.50 |
| 32:DL:70:ARG:NH1 | 32:DL:74:GLY:O | 2.45 | 0.50 |
| 53:DA:1420:A:C8 | 53:DA:2211:A:N6 | 2.80 | 0.50 |
| 32:CL:78:ARG:NH1 | 37:CQ:71:GLU:OE2 | 2.45 | 0.50 |
| 22:CA:1515:A:HO2' | 22:CA:1556:C:HO2' | 1.60 | 0.50 |
| 1:AA:109:A:C6 | 1:AA:326:G:C6 | 3.00 | 0.50 |
| 3:BC:3:GLN:N | 3:BC:3:GLN:OE1 | 2.45 | 0.50 |
| 1:BA:1047:G:HO2' | 1:BA:1215:G:HO2' | 1.56 | 0.50 |
| 53:DA:142:A:H1' | 41:DU:1:MET:HE1 | 1.92 | 0.49 |
| 42:CV:7:ARG:NH2 | 42:CV:8:ASP:OD1 | 2.40 | 0.49 |
| 1:BA:1491:G:C6 | 1:BA:1492:A:C6 | 3.00 | 0.49 |
| 32:DL:70:ARG:HD3 | 32:DL:76:VAL:HG22 | 1.93 | 0.49 |
| 13:AM:95:LEU:C | 13:AM:109:ARG:HG2 | 2.32 | 0.49 |
| 16:AP:1:MET:SD | 16:AP:1:MET:N | 2.64 | 0.49 |
| 41:CU:5:GLU:CG | 46:CZ:22:LEU:HD13 | 2.42 | 0.49 |
| 53:DA:2813:A:H2 | 53:DA:2887[B]:A:N1 | 2.10 | 0.49 |
| 22:CA:335:C:O2' | 22:CA:336:C:OP1 | 2.25 | 0.49 |
| 1:BA:1373:G:H5" | 7:BG:36:LYS:HB2 | 1.93 | 0.49 |
| 1:AA:1016:A:N1 | 1:AA:1017:U:O2' | 2.44 | 0.49 |
| 10:AJ:76:ILE:CD1 | 10:AJ:87:LEU:HD11 | 2.42 | 0.49 |
| 1:BA:674:G:N2 | 1:BA:717:U:O2 | 2.45 | 0.49 |
| 45:CY:11:ARG:HG2 | 45:CY:12:PRO:HD2 | 1.94 | 0.49 |
| 1:AA:266:G:H3' | 17:AQ:69:LYS:HB2 | 1.95 | 0.49 |
| 32:DL:113:MET:CE | 32:DL:116:ILE:HD11 | 2.41 | 0.49 |
| 19:AS:50:ALA:HB1 | 19:AS:57:HIS:HB3 | 1.93 | 0.49 |
| 22:CA:1262:A:C2 | 48:C1:7:LYS:HD2 | 2.47 | 0.49 |
| 22:CA:1340:U:C5 | 22:CA:1603:A:C8 | 3.00 | 0.49 |
| 33:DM:91:ASP:H | 33:DM:94:THR:HB | 1.78 | 0.49 |
| 15:BO:45:GLU:O | 15:BO:47:LYS:N | 2.44 | 0.49 |
| 3:BC:7:PRO:O | 3:BC:11:ARG:HG3 | 2.12 | 0.49 |
| 20:AT:44:LYS:HG3 | 20:AT:45:ALA:N | 2.27 | 0.49 |
| 17:BQ:81:LYS:N | 17:BQ:81:LYS:HD3 | 2.27 | 0.49 |
| 32:CL:99:ILE:HD13 | 32:CL:118:LEU:HB2 | 1.94 | 0.49 |
| 8:BH:59:LEU:HD12 | 8:BH:60:GLU:N | 2.26 | 0.49 |
| 1:AA:457:G:N2 | 1:AA:476:U:O2 | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:DG:2:SER:OG | 28:DG:6:LYS:NZ | 2.44 | 0.49 |
| 41:DU:2:ILE:HG21 | 41:DU:45:ALA:HB1 | 1.94 | 0.49 |
| 1:BA:842:U:N3 | 1:BA:844:G:H5' | 2.27 | 0.49 |
| 22:CA:2130:U:O2' | 22:CA:2133:G:O2' | 2.31 | 0.49 |
| 29:DH:41:LYS:HA | 29:DH:44:ILE:CG2 | 2.42 | 0.49 |
| 1:AA:1005:A:H3' | 1:AA:1006:G:C8 | 2.48 | 0.49 |
| 11:BK:43:GLY:HA3 | 11:BK:74:VAL:HG12 | 1.95 | 0.49 |
| 35:CO:28:LEU:O | 35:CO:32:GLU:N | 2.40 | 0.49 |
| 6:AF:29:ILE:HD13 | 6:AF:64:VAL:HG11 | 1.93 | 0.49 |
| 5:AE:156:LYS:NZ | 8:AH:73:GLU:OE1 | 2.45 | 0.49 |
| 1:BA:842:U:C2 | 1:BA:844:G:H5' | 2.48 | 0.49 |
| 22:CA:550:C:C2' | 22:CA:551:G:H5'' | 2.42 | 0.49 |
| 12:BL:82:ILE:HG12 | 12:BL:95:TYR:HB3 | 1.93 | 0.49 |
| 1:BA:79:G:N2 | 1:BA:91:U:N3 | 2.59 | 0.49 |
| 36:CP:49:VAL:HG21 | 36:CP:82:ALA:HA | 1.94 | 0.49 |
| 36:DP:31:THR:HG22 | 36:DP:34:HIS:H | 1.77 | 0.49 |
| 1:AA:147:G:H2' | 1:AA:148:G:C8 | 2.47 | 0.49 |
| 53:DA:2886[A]:A:C5 | 53:DA:2887[A]:A:N7 | 2.81 | 0.49 |
| 40:CT:96:ILE:H | 40:CT:96:ILE:HD13 | 1.77 | 0.49 |
| 12:BL:121:ARG:HG2 | 12:BL:121:ARG:HH11 | 1.77 | 0.49 |
| 1:BA:842:U:H3' | 1:BA:843:U:H5'' | 1.95 | 0.49 |
| 2:BB:120:GLN:HG3 | 2:BB:121:SER:N | 2.28 | 0.49 |
| 22:CA:374:A:C2 | 22:CA:401:A:C4 | 3.01 | 0.49 |
| 8:AH:9:ASP:OD1 | 8:AH:13:ARG:HD2 | 2.12 | 0.49 |
| 10:AJ:53:ILE:HG13 | 14:AN:85:ARG:CZ | 2.42 | 0.49 |
| 53:DA:1083:U:H4' | 55:DI:42:ARG:NH1 | 2.28 | 0.49 |
| 53:DA:1724:G:C2' | 53:DA:1725:U:H5' | 2.42 | 0.49 |
| 61:DQ:201:PEG:H22 | 69:DQ:313:HOH:O | 2.12 | 0.49 |
| 27:CF:135:GLN:OE1 | 27:CF:135:GLN:N | 2.46 | 0.49 |
| 6:BF:39:LEU:HD13 | 6:BF:62:MET:HG3 | 1.93 | 0.49 |
| 53:DA:933:A:H5' | 53:DA:934:U:OP2 | 2.12 | 0.49 |
| 1:BA:1381:U:C5 | 1:BA:1382:C:C5 | 3.01 | 0.49 |
| 38:DR:20:GLN:CG | 57:DR:202:PG4:H42 | 2.43 | 0.49 |
| 1:AA:71:A:O2' | 1:AA:72:A:OP2 | 2.27 | 0.49 |
| 36:CP:31:THR:HG22 | 36:CP:33:ARG:N | 2.28 | 0.49 |
| 1:AA:526:C:H2' | 1:AA:527:G7M:H5' | 1.93 | 0.49 |
| 22:CA:982:C:H5'' | 22:CA:983:A:OP1 | 2.13 | 0.49 |
| 1:BA:664:G:H22 | 1:BA:741:G:H1 | 1.61 | 0.49 |
| 53:DA:374:A:C2 | 53:DA:401:A:C4 | 3.01 | 0.49 |
| 11:BK:67:ALA:HB2 | 11:BK:96:THR:HG23 | 1.94 | 0.49 |
| 1:BA:976:G:OP2 | 1:BA:1358:U:O2' | 2.30 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:CE:127:GLU:O | 26:CE:156:ASN:ND2 | 2.46 | 0.49 |
| 53:DA:644:A:H2' | 53:DA:645:C:O4' | 2.12 | 0.49 |
| 54:DD:13:ARG:NH1 | 69:DD:479:HOH:O | 2.41 | 0.49 |
| 22:CA:2055:C:H5' | 22:CA:2056:G:OP1 | 2.13 | 0.49 |
| 19:BS:15:LEU:HD13 | 19:BS:33:THR:HG21 | 1.95 | 0.49 |
| 1:AA:184:G:O2' | 20:AT:69:LYS:NZ | 2.36 | 0.49 |
| 6:AF:86:ARG:NH1 | 18:AR:64:TYR:O | 2.46 | 0.49 |
| 1:BA:1516:2MG:N2 | 1:BA:1519:MA6:OP2 | 2.43 | 0.48 |
| 53:DA:1026:G:H2' | 53:DA:1027:A:C8 | 2.48 | 0.48 |
| 1:BA:958:A:N6 | 19:BS:77:THR:O | 2.46 | 0.48 |
| 1:AA:1238:A:H5' | 1:AA:1336:C:H41 | 1.77 | 0.48 |
| 5:AE:56:VAL:N | 5:AE:57:PRO:HD2 | 2.28 | 0.48 |
| 31:CK:81:ILE:HG12 | 31:CK:82:GLY:N | 2.27 | 0.48 |
| 6:AF:76:THR:O | 6:AF:79:ARG:N | 2.44 | 0.48 |
| 51:C4:62:LEU:HB3 | 51:C4:65:ALA:HB2 | 1.95 | 0.48 |
| 22:CA:627:A:OP1 | 33:CM:78:ARG:NH1 | 2.39 | 0.48 |
| 15:BO:18:ASP:OD1 | 15:BO:20:ASN:N | 2.28 | 0.48 |
| 14:BN:32:SER:HA | 14:BN:42:TRP:CZ2 | 2.48 | 0.48 |
| 7:BG:79:ARG:HA | 7:BG:83:SER:O | 2.13 | 0.48 |
| 1:BA:933:G:N7 | 7:BG:3:ARG:NH2 | 2.62 | 0.48 |
| 1:BA:754:C:OP1 | 15:BO:72:ARG:NH2 | 2.47 | 0.48 |
| 22:CA:377:G:C6 | 22:CA:378:C:C4 | 3.00 | 0.48 |
| 11:BK:107:ILE:HD11 | 11:BK:110:ILE:HG12 | 1.95 | 0.48 |
| 1:AA:975:A:H8 | 1:AA:1357:A:HO2' | 1.61 | 0.48 |
| 5:BE:106:ILE:O | 5:BE:106:ILE:HG13 | 2.13 | 0.48 |
| 13:BM:31:LYS:HA | 13:BM:31:LYS:HE3 | 1.93 | 0.48 |
| 53:DA:580:U:O3' | 38:DR:31:VAL:HG13 | 2.13 | 0.48 |
| 14:BN:10:GLU:HG3 | 14:BN:63:ARG:HD2 | 1.95 | 0.48 |
| 15:BO:4:SER:O | 15:BO:8:THR:HG23 | 2.13 | 0.48 |
| 35:CO:53:THR:HG1 | 35:CO:94:TYR:HH | 1.61 | 0.48 |
| 11:BK:16:VAL:HG13 | 11:BK:17:SER:N | 2.29 | 0.48 |
| 11:BK:16:VAL:HG13 | 11:BK:17:SER:H | 1.78 | 0.48 |
| 1:AA:1062:U:H2' | 1:AA:1063:C:C6 | 2.48 | 0.48 |
| 24:DC:130:LEU:CD1 | 24:DC:135:ILE:HG13 | 2.43 | 0.48 |
| 19:BS:50:ALA:HB1 | 19:BS:57:HIS:HB3 | 1.94 | 0.48 |
| 2:AB:120:GLN:HG3 | 2:AB:121:SER:N | 2.29 | 0.48 |
| 53:DA:1172:C:C5 | 53:DA:1173:U:C2 | 3.02 | 0.48 |
| 19:BS:11:ILE:HB | 19:BS:38:SER:HB3 | 1.95 | 0.48 |
| 29:CH:75:LEU:O | 29:CH:77:THR:N | 2.44 | 0.48 |
| 1:AA:131:A:H2' | 1:AA:132:C:C6 | 2.49 | 0.48 |
| 32:CL:35:VAL:HG22 | 32:CL:69:VAL:HG12 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:BA:890:G:O2' | 1:BA:906:A:N6 | 2.47 | 0.48 |
| 22:CA:1309:G:H4' | 50:C3:7:PRO:HB2 | 1.95 | 0.48 |
| 51:C4:45:ARG:N | 51:C4:46:PRO:HD2 | 2.29 | 0.48 |
| 18:BR:34:THR:HG22 | 18:BR:38:LYS:HB2 | 1.95 | 0.48 |
| 6:BF:73:GLU:O | 6:BF:77:THR:OG1 | 2.31 | 0.48 |
| 33:CM:82:LEU:HD23 | 33:CM:83:ALA:N | 2.28 | 0.48 |
| 2:AB:15:HIS:HB3 | 2:AB:43:LEU:HD11 | 1.95 | 0.48 |
| 1:BA:380:G:N2 | 1:BA:383:A:OP2 | 2.45 | 0.48 |
| 1:BA:1302:C:C5 | 13:BM:17:ILE:HD11 | 2.49 | 0.48 |
| 1:BA:841:C:H5' | 1:BA:842:U:OP2 | 2.13 | 0.48 |
| 14:BN:28:LYS:HA | 14:BN:31:ILE:HG22 | 1.96 | 0.48 |
| 24:CC:160:THR:HG22 | 24:CC:177:ARG:HG2 | 1.94 | 0.48 |
| 3:BC:45:LYS:HG3 | 3:BC:46:GLU:N | 2.28 | 0.48 |
| 12:BL:56:ARG:HG3 | 12:BL:62:GLU:HB2 | 1.95 | 0.48 |
| 22:CA:1638:C:O2 | 22:CA:2698:U:O2' | 2.24 | 0.48 |
| 1:AA:429:U:H5' | 4:AD:9:LEU:HD12 | 1.95 | 0.48 |
| 59:DA:3214:PUT:H32 | 69:DA:8098:HOH:O | 2.14 | 0.48 |
| 22:CA:618:G:O6 | 69:CA:3267:HOH:O | 2.19 | 0.48 |
| 1:AA:383:A:C5 | 1:AA:384:G:H1' | 2.49 | 0.48 |
| 22:CA:991:C:H5' | 22:CA:1186:G:H5' | 1.95 | 0.48 |
| 29:DH:42:LYS:HG2 | 29:DH:43:ASN:N | 2.28 | 0.48 |
| 22:CA:2489:U:HO2' | 22:CA:2491:U:H5 | 1.61 | 0.48 |
| 14:AN:10:GLU:HG3 | 14:AN:63:ARG:HD2 | 1.96 | 0.48 |
| 22:CA:2599:G:N7 | 24:CC:236:GLU:HB2 | 2.28 | 0.48 |
| 22:CA:2604:U:O2 | 69:CA:3811:HOH:O | 2.16 | 0.48 |
| 22:CA:1616:A:O2' | 69:CA:3372:HOH:O | 2.20 | 0.48 |
| 8:BH:29:SER:HB3 | 8:BH:57:PRO:HB2 | 1.95 | 0.48 |
| 23:DB:90:C:H5'' | 23:DB:90:C:H6 | 1.77 | 0.48 |
| 1:AA:1137:C:H1' | 1:AA:1138:G:N2 | 2.28 | 0.48 |
| 12:BL:14:ARG:CA | 12:BL:14:ARG:HH11 | 2.26 | 0.48 |
| 19:BS:10:PHE:CG | 19:BS:11:ILE:N | 2.82 | 0.48 |
| 1:AA:973:G:H1' | 10:AJ:56:HIS:HD2 | 1.78 | 0.48 |
| 5:BE:81:LEU:CD1 | 5:BE:120:VAL:HG11 | 2.43 | 0.48 |
| 5:BE:81:LEU:O | 5:BE:98:PRO:HB3 | 2.13 | 0.48 |
| 13:AM:40:ALA:HB3 | 13:AM:43:VAL:CG2 | 2.43 | 0.48 |
| 43:CW:38:LEU:HG | 43:CW:40:ILE:HD13 | 1.95 | 0.48 |
| 1:AA:900:A:OP2 | 69:AA:2151:HOH:O | 2.20 | 0.48 |
| 53:DA:2086:U:H2' | 53:DA:2087:G:C8 | 2.49 | 0.48 |
| 36:CP:43:ASN:ND2 | 36:CP:46:GLU:OE1 | 2.42 | 0.48 |
| 14:BN:31:ILE:HA | 14:BN:34:VAL:HG23 | 1.94 | 0.48 |
| 14:BN:45:VAL:HG12 | 19:BS:10:PHE:HE1 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 39:CS:39:LEU:O | 39:CS:49:ILE:HG23 | 2.14 | 0.48 |
| 2:AB:133:GLU:OE2 | 2:AB:137:ARG:NH1 | 2.39 | 0.48 |
| 27:CF:42:GLU:OE1 | 27:CF:148:ARG:NH2 | 2.47 | 0.48 |
| 1:BA:376:G:H5'' | 16:BP:5:ARG:HB2 | 1.96 | 0.48 |
| 34:DN:47:GLU:OE2 | 34:DN:51:ARG:NE | 2.46 | 0.48 |
| 10:AJ:53:ILE:CG2 | 10:AJ:61:ALA:HB1 | 2.44 | 0.48 |
| 1:AA:1016:A:C2 | 1:AA:1017:U:H4' | 2.48 | 0.48 |
| 28:CG:80:THR:CG2 | 28:CG:81:GLU:N | 2.77 | 0.48 |
| 1:BA:510:A:C5' | 1:BA:511:C:P | 3.01 | 0.48 |
| 53:DA:837:C:N4 | 69:DA:6883:HOH:O | 2.47 | 0.48 |
| 22:CA:1714:U:H5'' | 22:CA:1715:G:H5' | 1.95 | 0.48 |
| 13:AM:107:ARG:HH21 | 13:AM:113:ARG:HB3 | 1.79 | 0.48 |
| 5:AE:162:GLU:HG3 | 5:AE:163:GLU:N | 2.28 | 0.48 |
| 22:CA:1339:G:N2 | 22:CA:1603:A:N3 | 2.62 | 0.48 |
| 10:BJ:17:LEU:HD11 | 10:BJ:94:ALA:HB3 | 1.95 | 0.48 |
| 55:DI:66:GLY:O | 55:DI:67:THR:CB | 2.62 | 0.48 |
| 6:BF:86:ARG:CG | 6:BF:86:ARG:HH11 | 2.27 | 0.48 |
| 1:BA:159:G:N2 | 1:BA:161:A:H3' | 2.29 | 0.48 |
| 27:CF:38:MET:HG2 | 27:CF:152:LEU:HB3 | 1.96 | 0.48 |
| 53:DA:137:U:H2' | 53:DA:140:C:C1' | 2.44 | 0.48 |
| 1:AA:1003:G:N2 | 1:AA:1004:A:O2' | 2.46 | 0.48 |
| 27:DF:40:VAL:HG11 | 27:DF:43:ALA:HB2 | 1.95 | 0.48 |
| 53:DA:1342:A:OP1 | 41:DU:40:LYS:NZ | 2.40 | 0.48 |
| 19:BS:29:LYS:CB | 19:BS:30:PRO:HD2 | 2.44 | 0.48 |
| 1:BA:1492:A:N7 | 1:BA:1493:A:C2 | 2.82 | 0.48 |
| 30:DJ:21:SER:HB3 | 30:DJ:22:PRO:HD3 | 1.96 | 0.48 |
| 53:DA:2251:OMG:HM23 | 53:DA:2251:OMG:H1' | 1.67 | 0.48 |
| 22:CA:563:A:N3 | 38:CR:37:GLN:NE2 | 2.61 | 0.48 |
| 42:CV:54:GLN:N | 42:CV:55:PRO:HD3 | 2.28 | 0.48 |
| 4:AD:17:THR:HG22 | 4:AD:18:ASP:N | 2.29 | 0.48 |
| 22:CA:818:G:O2' | 22:CA:819:A:O4' | 2.27 | 0.48 |
| 22:CA:2020:A:H5' | 48:C1:9:THR:CG2 | 2.44 | 0.48 |
| 53:DA:2609:U:H5 | 66:DA:3194:EDO:H12 | 1.74 | 0.47 |
| 42:CV:74:ASN:O | 42:CV:74:ASN:ND2 | 2.44 | 0.47 |
| 14:BN:42:TRP:CE2 | 14:BN:44:ALA:HB3 | 2.49 | 0.47 |
| 22:CA:1339:G:OP1 | 41:CU:17:SER:OG | 2.30 | 0.47 |
| 53:DA:1105:U:H2' | 53:DA:1106:G:C8 | 2.49 | 0.47 |
| 58:DA:3205:MPD:C5 | 58:DA:3205:MPD:HM2 | 2.44 | 0.47 |
| 53:DA:811:U:H2' | 33:DM:21:ARG:HA | 1.96 | 0.47 |
| 1:BA:205:A:N1 | 1:BA:206:C:N4 | 2.62 | 0.47 |
| 53:DA:2305:U:C2 | 27:DF:151:GLY:HA3 | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:BA:121:U:H5'' | 1:BA:122:G:OP2 | 2.14 | 0.47 |
| 38:CR:78:LYS:HE2 | 38:CR:117:LEU:HD21 | 1.95 | 0.47 |
| 5:AE:94:VAL:HG22 | 5:AE:111:MET:CE | 2.44 | 0.47 |
| 27:CF:20:PHE:HB2 | 27:CF:22:TYR:CE1 | 2.49 | 0.47 |
| 22:CA:1497:U:OP2 | 22:CA:1498:C:N4 | 2.46 | 0.47 |
| 22:CA:17:G:H4' | 38:CR:25:TYR:CE2 | 2.48 | 0.47 |
| 29:CH:51:ARG:HG3 | 29:CH:52:ALA:N | 2.28 | 0.47 |
| 53:DA:2813:A:H2 | 53:DA:2887[B]:A:C6 | 2.31 | 0.47 |
| 1:AA:1429:A:O2' | 53:DA:1703:G:O3' | 2.32 | 0.47 |
| 10:AJ:8:ILE:HA | 10:AJ:99:GLN:O | 2.14 | 0.47 |
| 53:DA:2291:U:H2' | 53:DA:2292:U:C6 | 2.49 | 0.47 |
| 53:DA:545:U:H3' | 53:DA:546:U:H4' | 1.95 | 0.47 |
| 30:DJ:22:PRO:HB2 | 30:DJ:23:PRO:HD3 | 1.96 | 0.47 |
| 11:AK:16:VAL:HG23 | 11:AK:17:SER:N | 2.28 | 0.47 |
| 31:CK:37:ARG:NH2 | 31:CK:44:TYR:OH | 2.47 | 0.47 |
| 22:CA:223:A:O2' | 22:CA:420:C:O2 | 2.30 | 0.47 |
| 22:CA:249:C:H5' | 22:CA:2394:C:O2' | 2.13 | 0.47 |
| 1:AA:913:A:OP1 | 12:AL:88:LYS:NZ | 2.47 | 0.47 |
| 22:CA:2200:C:O2 | 22:CA:2226:C:N4 | 2.47 | 0.47 |
| 53:DA:1847:A:H8 | 53:DA:1847:A:O5' | 1.98 | 0.47 |
| 53:DA:2162:G:H5'' | 53:DA:2171:A:H2' | 1.95 | 0.47 |
| 26:CE:52:VAL:HG21 | 26:CE:81:GLY:HA2 | 1.95 | 0.47 |
| 5:BE:26:LYS:CA | 5:BE:26:LYS:HE3 | 2.44 | 0.47 |
| 5:BE:81:LEU:HB3 | 5:BE:147:MET:SD | 2.54 | 0.47 |
| 14:AN:42:TRP:CD1 | 14:AN:43:ASN:N | 2.83 | 0.47 |
| 1:AA:159:G:H8 | 1:AA:159:G:H5'' | 1.79 | 0.47 |
| 22:CA:118:A:N3 | 22:CA:178:G:H1' | 2.29 | 0.47 |
| 45:CY:72:ARG:CZ | 45:CY:72:ARG:HB2 | 2.45 | 0.47 |
| 42:CV:13:VAL:HG21 | 42:CV:39:ILE:CG2 | 2.44 | 0.47 |
| 10:AJ:51:VAL:HB | 14:AN:81:ARG:HB2 | 1.96 | 0.47 |
| 53:DA:2534:A:H2' | 53:DA:2535:G:O5' | 2.14 | 0.47 |
| 33:CM:29:LYS:C | 33:CM:31:GLY:H | 2.17 | 0.47 |
| 23:DB:28:C:OP1 | 36:DP:31:THR:HG21 | 2.15 | 0.47 |
| 29:DH:43:ASN:O | 29:DH:46:PHE:HB3 | 2.15 | 0.47 |
| 22:CA:558:U:H1' | 31:CK:47:HIS:HB3 | 1.96 | 0.47 |
| 1:BA:411:A:P | 4:BD:26:ARG:HH12 | 2.38 | 0.47 |
| 53:DA:1378:A:O2' | 53:DA:1380:G:N7 | 2.47 | 0.47 |
| 53:DA:1971:U:H4' | 53:DA:1971:U:OP2 | 2.14 | 0.47 |
| 53:DA:1582:C:C4 | 53:DA:1583:A:C2 | 3.02 | 0.47 |
| 1:AA:26:A:H2' | 1:AA:27:G:H5' | 1.95 | 0.47 |
| 55:DI:68:PRO:HD2 | 55:DI:69:PHE:CE2 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:BA:455:G:C2 | 1:BA:478:A:C2 | 3.02 | 0.47 |
| 9:AI:23:PRO:HA | 9:AI:61:LEU:HA | 1.95 | 0.47 |
| 13:AM:33:ILE:HD11 | 13:AM:63:PHE:CE1 | 2.50 | 0.47 |
| 22:CA:820:A:N6 | 69:CA:3772:HOH:O | 2.43 | 0.47 |
| 22:CA:647:G:N2 | 22:CA:2350:C:O3' | 2.48 | 0.47 |
| 53:DA:289:G:H2' | 53:DA:290:U:O4' | 2.14 | 0.47 |
| 59:DA:3222:PUT:H11 | 59:DA:3222:PUT:H41 | 1.47 | 0.47 |
| 39:CS:8:GLY:O | 39:CS:10:LYS:NZ | 2.39 | 0.47 |
| 53:DA:871:U:H2' | 53:DA:872:U:C6 | 2.50 | 0.47 |
| 24:DC:125:LYS:HB2 | 24:DC:126:PRO:HD2 | 1.96 | 0.47 |
| 9:BI:36:GLU:HA | 9:BI:45:ARG:HE | 1.79 | 0.47 |
| 22:CA:1178:C:C2 | 22:CA:1179:G:N7 | 2.82 | 0.47 |
| 35:CO:8:ARG:HB3 | 35:CO:10:LEU:HG | 1.95 | 0.47 |
| 53:DA:1171:G:H3' | 53:DA:1172:C:C5 | 2.50 | 0.47 |
| 53:DA:1171:G:N3 | 53:DA:1179:G:C2 | 2.83 | 0.47 |
| 1:AA:1228:C:P | 13:AM:107:ARG:NH2 | 2.88 | 0.47 |
| 53:DA:2286:G:OP1 | 49:D2:30:LYS:NZ | 2.37 | 0.47 |
| 1:AA:207:C:H2' | 1:AA:208:U:C2 | 2.49 | 0.47 |
| 13:BM:93:ARG:NH2 | 19:BS:80:TYR:CE1 | 2.82 | 0.47 |
| 36:CP:34:HIS:N | 36:CP:65:THR:O | 2.47 | 0.47 |
| 30:DJ:19:ASN:N | 30:DJ:20:PRO:HD2 | 2.29 | 0.47 |
| 53:DA:2498:OMC:HM22 | 53:DA:2499:C:O4' | 2.15 | 0.47 |
| 53:DA:281:C:H2' | 53:DA:282:A:C8 | 2.50 | 0.47 |
| 22:CA:2019:A:H4' | 38:CR:34:VAL:HG21 | 1.96 | 0.47 |
| 22:CA:818:G:H2' | 22:CA:819:A:H5'' | 1.97 | 0.47 |
| 59:DA:3222:PUT:H42 | 69:DL:343:HOH:O | 2.13 | 0.47 |
| 29:CH:68:ARG:NH1 | 29:CH:114:GLU:OE1 | 2.48 | 0.47 |
| 1:BA:765:G:C6 | 1:BA:812:G:C4 | 3.02 | 0.47 |
| 22:CA:2674:G:H4' | 32:CL:30:ARG:HD2 | 1.97 | 0.47 |
| 53:DA:493:G:H2' | 53:DA:494:G:O4' | 2.14 | 0.47 |
| 5:AE:80:THR:OG1 | 5:AE:122:ASN:O | 2.32 | 0.47 |
| 1:AA:944:G:N1 | 1:AA:1338:G:OP2 | 2.41 | 0.47 |
| 18:AR:21:ILE:HG21 | 18:AR:54:GLN:HB3 | 1.95 | 0.47 |
| 22:CA:621:A:OP2 | 33:CM:99:ASN:ND2 | 2.45 | 0.47 |
| 23:CB:23:G:O6 | 69:CB:304:HOH:O | 2.19 | 0.47 |
| 6:AF:14:GLN:NE2 | 4:BD:166:GLU:OE1 | 2.48 | 0.47 |
| 53:DA:1475:G:H5' | 69:DA:4930:HOH:O | 2.14 | 0.47 |
| 22:CA:2379:G:H4' | 36:CP:21:LEU:HD11 | 1.97 | 0.47 |
| 7:BG:42:ILE:HG21 | 7:BG:116:MET:HG3 | 1.96 | 0.47 |
| 7:BG:4:ARG:HG3 | 7:BG:5:ARG:N | 2.29 | 0.47 |
| 2:AB:20:THR:HG22 | 2:AB:39:HIS:CE1 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 53:DA:1714:U:H5'' | 53:DA:1715:G:H5' | 1.97 | 0.47 |
| 15:AO:89:ARG:NH1 | 53:DA:716:A:OP1 | 2.48 | 0.47 |
| 15:AO:89:ARG:NH1 | 53:DA:716:A:P | 2.88 | 0.47 |
| 13:BM:14:HIS:HB2 | 13:BM:17:ILE:HD12 | 1.97 | 0.47 |
| 30:DJ:113:LYS:O | 30:DJ:117:MET:HG2 | 2.15 | 0.47 |
| 24:CC:260:ASN:C | 24:CC:262:ARG:H | 2.18 | 0.47 |
| 10:AJ:7:ARG:CG | 10:AJ:101:SER:HB2 | 2.44 | 0.47 |
| 22:CA:1581:G:C6 | 22:CA:1582:C:C4 | 3.03 | 0.47 |
| 3:BC:7:PRO:HG2 | 3:BC:184:TYR:CG | 2.50 | 0.47 |
| 53:DA:1133:A:N3 | 59:DA:3214:PUT:H22 | 2.30 | 0.47 |
| 42:CV:39:ILE:O | 42:CV:39:ILE:HG22 | 2.14 | 0.47 |
| 55:DI:29:ASP:OD1 | 55:DI:30:SER:N | 2.48 | 0.47 |
| 1:BA:1394:A:C5 | 1:BA:1501:C:H4' | 2.49 | 0.47 |
| 49:C2:11:LEU:HA | 49:C2:50:LYS:O | 2.15 | 0.47 |
| 41:CU:8:LEU:O | 46:CZ:29:ARG:NH1 | 2.46 | 0.47 |
| 2:BB:217:VAL:O | 2:BB:221:VAL:HG23 | 2.15 | 0.47 |
| 30:DJ:12:GLN:HA | 30:DJ:56:PRO:HA | 1.97 | 0.47 |
| 8:AH:108:LYS:HG3 | 8:AH:121:LEU:HD11 | 1.97 | 0.47 |
| 22:CA:1246:A:O2' | 26:CE:40:ARG:NH2 | 2.47 | 0.47 |
| 33:DM:57:LEU:HD22 | 51:D4:54:ASP:HB3 | 1.97 | 0.47 |
| 53:DA:1309:G:H4' | 50:D3:7:PRO:HB2 | 1.96 | 0.47 |
| 9:AI:19:VAL:HG13 | 9:AI:65:ILE:HG22 | 1.97 | 0.47 |
| 29:CH:72:ILE:HG23 | 29:CH:142:VAL:HG22 | 1.97 | 0.47 |
| 4:BD:107:PHE:CG | 4:BD:145:ILE:HD11 | 2.50 | 0.47 |
| 33:CM:77:ILE:HG23 | 33:CM:100:ILE:HD11 | 1.96 | 0.47 |
| 5:BE:136:VAL:O | 5:BE:138:ARG:N | 2.47 | 0.47 |
| 13:BM:8:ASN:O | 13:BM:10:PRO:HD2 | 2.15 | 0.47 |
| 1:AA:76:G:N3 | 1:AA:76:G:H2' | 2.29 | 0.47 |
| 53:DA:1555:G:OP1 | 59:DA:3220:PUT:H41 | 2.13 | 0.47 |
| 17:BQ:10:GLY:HA3 | 17:BQ:25:ILE:HD13 | 1.97 | 0.47 |
| 11:BK:49:GLY:O | 11:BK:69:ARG:NH2 | 2.48 | 0.47 |
| 22:CA:668:A:H2' | 22:CA:670:A:H62 | 1.80 | 0.47 |
| 22:CA:574:A:H4' | 22:CA:575:A:C5' | 2.45 | 0.47 |
| 7:AG:130:ASN:HA | 7:AG:135:VAL:HG11 | 1.96 | 0.47 |
| 11:BK:97:ILE:HD11 | 21:BU:16:LEU:HG | 1.96 | 0.47 |
| 22:CA:751:A:C6 | 22:CA:789:A:C6 | 3.03 | 0.47 |
| 38:DR:19:LYS:CD | 57:DR:202:PG4:H41 | 2.43 | 0.47 |
| 12:BL:14:ARG:NH1 | 12:BL:15:LYS:H | 2.13 | 0.47 |
| 22:CA:514:A:N3 | 22:CA:581:C:O2' | 2.41 | 0.47 |
| 1:BA:1376:U:H2' | 1:BA:1377:A:C8 | 2.50 | 0.47 |
| 32:CL:38:ILE:HD11 | 32:CL:112:PHE:CZ | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:BB:117:LEU:HA | 2:BB:120:GLN:HG2 | 1.97 | 0.47 |
| 2:AB:129:LEU:HD22 | 2:AB:134:ALA:HB2 | 1.97 | 0.47 |
| 53:DA:137:U:H5'' | 53:DA:140:C:C4 | 2.50 | 0.47 |
| 1:AA:75:G:C2 | 1:AA:76:G:H1' | 2.50 | 0.47 |
| 29:CH:135:HIS:CG | 29:CH:136:SER:H | 2.32 | 0.47 |
| 28:DG:86:LYS:HG2 | 28:DG:132:VAL:HG22 | 1.97 | 0.47 |
| 1:BA:1053:G:N7 | 1:BA:1199:U:H3' | 2.30 | 0.47 |
| 13:BM:114:LYS:CB | 13:BM:115:PRO:HD3 | 2.45 | 0.47 |
| 22:CA:135:U:H3 | 22:CA:144:A:H61 | 1.61 | 0.47 |
| 1:BA:1345:U:H4' | 1:BA:1346:A:H5' | 1.97 | 0.47 |
| 1:AA:451:A:H61 | 1:AA:481:G:H5' | 1.80 | 0.47 |
| 22:CA:1061:U:OP2 | 30:CJ:10:LYS:NZ | 2.48 | 0.47 |
| 3:BC:19:ASN:ND2 | 14:BN:90:ARG:O | 2.47 | 0.47 |
| 3:AC:185:ASN:OD1 | 3:AC:186:THR:N | 2.45 | 0.47 |
| 53:DA:435:C:H2' | 53:DA:436:C:H5' | 1.96 | 0.47 |
| 22:CA:545:U:H2' | 22:CA:547:A:H5' | 1.96 | 0.47 |
| 14:BN:32:SER:HB2 | 14:BN:42:TRP:NE1 | 2.30 | 0.46 |
| 22:CA:1869:G:H3' | 22:CA:1870:C:C5' | 2.45 | 0.46 |
| 22:CA:1585:C:C2' | 22:CA:1586:A:H5' | 2.45 | 0.46 |
| 1:AA:109:A:H2' | 1:AA:326:G:N2 | 2.31 | 0.46 |
| 53:DA:137:U:C6 | 53:DA:140:C:H1' | 2.51 | 0.46 |
| 3:BC:185:ASN:OD1 | 3:BC:186:THR:N | 2.47 | 0.46 |
| 6:AF:102:MET:CE | 18:AR:24:LYS:HB3 | 2.45 | 0.46 |
| 42:CV:4:LYS:O | 42:CV:94:ARG:NH2 | 2.42 | 0.46 |
| 1:AA:1464:U:P | 37:DQ:109:ARG:HH12 | 2.38 | 0.46 |
| 51:D4:42:ARG:NH2 | 69:D4:113:HOH:O | 2.48 | 0.46 |
| 2:BB:28:LYS:N | 2:BB:29:PRO:CD | 2.78 | 0.46 |
| 22:CA:1081:U:H4' | 30:CJ:124:ALA:HB1 | 1.96 | 0.46 |
| 15:BO:20:ASN:O | 15:BO:22:THR:N | 2.46 | 0.46 |
| 53:DA:545:U:H6 | 53:DA:548:G:P | 2.38 | 0.46 |
| 1:AA:1229:A:OP2 | 13:AM:113:ARG:NH1 | 2.48 | 0.46 |
| 14:AN:21:PHE:HA | 14:AN:25:ALA:CB | 2.45 | 0.46 |
| 14:BN:42:TRP:NE1 | 14:BN:44:ALA:HB3 | 2.30 | 0.46 |
| 30:DJ:20:PRO:HB2 | 30:DJ:23:PRO:HD2 | 1.97 | 0.46 |
| 10:AJ:35:GLN:HG3 | 10:AJ:78:GLU:HG2 | 1.98 | 0.46 |
| 37:DQ:112:GLU:HG2 | 37:DQ:114:LEU:HG | 1.96 | 0.46 |
| 8:AH:3:MET:N | 8:AH:3:MET:SD | 2.73 | 0.46 |
| 19:AS:7:LYS:HD2 | 19:AS:7:LYS:H | 1.79 | 0.46 |
| 41:DU:92:ASN:O | 41:DU:93:LEU:HB2 | 2.16 | 0.46 |
| 7:BG:50:LEU:CD1 | 7:BG:61:ALA:HB1 | 2.45 | 0.46 |
| 24:DC:227:PRO:HA | 24:DC:233:GLY:HA2 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 53:DA:1700:A:N1 | 69:DA:6711:HOH:O | 2.36 | 0.46 |
| 66:DA:3198:EDO:H12 | 64:DA:3204:PGE:C3 | 2.42 | 0.46 |
| 11:BK:98:ARG:HA | 21:BU:12:PHE:CZ | 2.51 | 0.46 |
| 19:BS:30:PRO:HB2 | 19:BS:50:ALA:HB2 | 1.97 | 0.46 |
| 30:CJ:19:ASN:HA | 30:CJ:39:CYS:SG | 2.55 | 0.46 |
| 22:CA:223:A:N1 | 22:CA:407:G:O2' | 2.41 | 0.46 |
| 10:BJ:5:ARG:HB3 | 10:BJ:77:VAL:HG13 | 1.97 | 0.46 |
| 5:BE:11:LEU:HG | 5:BE:12:GLN:N | 2.30 | 0.46 |
| 48:D1:2:ALA:N | 69:D1:204:HOH:O | 2.48 | 0.46 |
| 7:AG:62:PHE:HE2 | 7:AG:66:LEU:HD22 | 1.81 | 0.46 |
| 1:BA:677:U:H3 | 1:BA:713:G:H22 | 1.62 | 0.46 |
| 11:BK:14:LYS:O | 11:BK:15:GLN:HB3 | 2.16 | 0.46 |
| 10:AJ:42:LEU:HB2 | 10:AJ:71:LEU:HB3 | 1.96 | 0.46 |
| 29:CH:31:VAL:HB | 29:CH:32:PRO:HD3 | 1.97 | 0.46 |
| 42:DV:73:PHE:CE2 | 42:DV:75:ALA:HA | 2.51 | 0.46 |
| 53:DA:1161:C:O2' | 39:DS:8:GLY:HA2 | 2.14 | 0.46 |
| 53:DA:961:C:H5' | 63:DA:3203:1PE:H222 | 1.98 | 0.46 |
| 53:DA:2256:G:N3 | 57:DA:3193:PG4:H31 | 2.29 | 0.46 |
| 1:BA:502:A:H2' | 1:BA:503:C:O4' | 2.15 | 0.46 |
| 53:DA:483:A:H2' | 53:DA:484:C:H5' | 1.96 | 0.46 |
| 22:CA:846:U:O2' | 22:CA:847:U:P | 2.74 | 0.46 |
| 22:CA:2790:U:H4' | 22:CA:2791:G:OP1 | 2.15 | 0.46 |
| 40:CT:62:ASP:N | 40:CT:62:ASP:OD1 | 2.49 | 0.46 |
| 1:AA:1018:G:N3 | 1:AA:1018:G:H2' | 2.30 | 0.46 |
| 54:DD:99:GLU:HG2 | 54:DD:182:ALA:HB2 | 1.98 | 0.46 |
| 10:AJ:22:THR:CG2 | 10:AJ:39:PRO:HB3 | 2.46 | 0.46 |
| 22:CA:2271:G:O6 | 69:CA:3441:HOH:O | 2.21 | 0.46 |
| 49:D2:22:THR:OG1 | 51:D4:34:THR:OG1 | 2.26 | 0.46 |
| 1:AA:468:A:C8 | 1:AA:469:C:C6 | 3.03 | 0.46 |
| 24:CC:233:GLY:H | 24:CC:242:LYS:HE3 | 1.81 | 0.46 |
| 13:AM:6:GLY:HA3 | 13:AM:66:GLU:HG3 | 1.97 | 0.46 |
| 13:AM:54:ASP:HA | 13:AM:57:ARG:HD2 | 1.98 | 0.46 |
| 16:BP:79:ASN:O | 16:BP:80:LYS:HG3 | 2.15 | 0.46 |
| 50:C3:43:THR:OG1 | 50:C3:44:VAL:N | 2.48 | 0.46 |
| 22:CA:1808:A:N1 | 45:CY:28:ARG:HD2 | 2.31 | 0.46 |
| 1:AA:1152:A:H5'' | 10:AJ:15:HIS:HB2 | 1.97 | 0.46 |
| 9:AI:19:VAL:HG11 | 9:AI:83:ILE:HA | 1.98 | 0.46 |
| 1:BA:1299:A:N3 | 1:BA:1299:A:H2' | 2.31 | 0.46 |
| 55:DI:54:VAL:HG22 | 55:DI:81:LEU:HD13 | 1.96 | 0.46 |
| 25:CD:121:THR:HB | 25:CD:127:PHE:CD2 | 2.51 | 0.46 |
| 6:BF:76:THR:O | 6:BF:79:ARG:N | 2.47 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:CA:747:5MU:O2 | 22:CA:2014:A:H1' | 2.15 | 0.46 |
| 1:AA:1492:A:H4' | 12:AL:44:LYS:HE2 | 1.97 | 0.46 |
| 14:BN:22:ALA:C | 14:BN:26:GLU:OE1 | 2.53 | 0.46 |
| 1:AA:1134:G:H2' | 1:AA:1135:U:C6 | 2.51 | 0.46 |
| 53:DA:845:A:H5' | 53:DA:846:U:OP2 | 2.15 | 0.46 |
| 13:BM:93:ARG:NH2 | 19:BS:80:TYR:HE1 | 2.13 | 0.46 |
| 32:CL:76:VAL:HG22 | 37:CQ:73:VAL:HG23 | 1.97 | 0.46 |
| 22:CA:1853:A:N6 | 22:CA:1888:G:O2' | 2.48 | 0.46 |
| 34:DN:21:ALA:HB1 | 34:DN:100:LYS:HG3 | 1.98 | 0.46 |
| 23:CB:8:C:O3' | 36:CP:25:ARG:NH1 | 2.48 | 0.46 |
| 24:CC:217:ARG:HB3 | 24:CC:218:PRO:HD2 | 1.97 | 0.46 |
| 24:CC:117:GLN:N | 24:CC:128:ASN:OD1 | 2.48 | 0.46 |
| 25:CD:113:SER:HB3 | 25:CD:170:VAL:HG21 | 1.98 | 0.46 |
| 29:CH:1:MET:SD | 29:CH:27:ARG:NH1 | 2.89 | 0.46 |
| 22:CA:1820:U:C4 | 24:CC:159:GLY:HA3 | 2.50 | 0.46 |
| 14:BN:45:VAL:HG12 | 19:BS:10:PHE:CE1 | 2.50 | 0.46 |
| 7:BG:16:PRO:HB2 | 9:BI:46:MET:SD | 2.56 | 0.46 |
| 5:BE:81:LEU:HD12 | 5:BE:120:VAL:HG11 | 1.97 | 0.46 |
| 10:AJ:15:HIS:CG | 10:AJ:16:ARG:N | 2.84 | 0.46 |
| 53:DA:1738:G:HO2' | 53:DA:1739:A:H8 | 1.63 | 0.46 |
| 50:C3:30:VAL:O | 50:C3:34:ARG:HG3 | 2.15 | 0.46 |
| 1:AA:254:G:H4' | 17:AQ:17:MET:HE2 | 1.98 | 0.46 |
| 3:AC:123:GLN:HG2 | 3:AC:128:VAL:HG21 | 1.97 | 0.46 |
| 55:DI:82:ILE:HD12 | 55:DI:84:TYR:CE2 | 2.51 | 0.46 |
| 42:CV:51:ALA:O | 42:CV:52:LEU:HB2 | 2.16 | 0.46 |
| 7:AG:83:SER:HB2 | 7:AG:85:TYR:CE2 | 2.51 | 0.46 |
| 53:DA:139:U:O2' | 53:DA:141:G:N1 | 2.44 | 0.46 |
| 1:BA:1004:A:C2 | 1:BA:1026:G:C2 | 3.04 | 0.46 |
| 25:CD:149:ASN:O | 25:CD:151:THR:O | 2.33 | 0.46 |
| 1:BA:532:A:N3 | 1:BA:532:A:H2' | 2.30 | 0.46 |
| 2:AB:126:PHE:CG | 2:AB:127:ASP:N | 2.84 | 0.46 |
| 14:AN:21:PHE:HB2 | 14:AN:55:SER:O | 2.16 | 0.46 |
| 20:AT:44:LYS:HB3 | 20:AT:87:ALA:HB3 | 1.98 | 0.46 |
| 42:CV:13:VAL:HG21 | 42:CV:39:ILE:HG23 | 1.98 | 0.46 |
| 12:BL:43:LYS:HD2 | 12:BL:91:PRO:HG3 | 1.97 | 0.46 |
| 22:CA:1274:A:N3 | 22:CA:1297:C:H1' | 2.30 | 0.46 |
| 5:BE:56:VAL:N | 5:BE:57:PRO:HD2 | 2.31 | 0.46 |
| 53:DA:1585:C:H2' | 53:DA:1586:A:O4' | 2.15 | 0.46 |
| 27:CF:40:VAL:HG11 | 27:CF:50:LEU:HD13 | 1.98 | 0.46 |
| 22:CA:533:G:H5' | 38:CR:24:TYR:CE1 | 2.51 | 0.46 |
| 22:CA:1783:A:H5' | 22:CA:2608:G:H4' | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DC:31:ALA:HB3 | 24:DC:32:PRO:HD3 | 1.97 | 0.46 |
| 25:CD:97:SER:OG | 25:CD:98:VAL:N | 2.49 | 0.46 |
| 14:BN:23:LYS:C | 14:BN:26:GLU:OE2 | 2.54 | 0.46 |
| 5:BE:154:ALA:O | 5:BE:156:LYS:N | 2.36 | 0.46 |
| 15:BO:89:ARG:HH12 | 22:CA:716:A:P | 2.39 | 0.46 |
| 18:BR:34:THR:CG2 | 18:BR:38:LYS:HB2 | 2.45 | 0.46 |
| 1:BA:510:A:H5'' | 1:BA:511:C:OP2 | 2.16 | 0.46 |
| 50:C3:3:ARG:NE | 50:C3:3:ARG:HA | 2.31 | 0.46 |
| 2:BB:62:SER:HB2 | 2:BB:227:GLN:HG3 | 1.97 | 0.46 |
| 22:CA:1794:A:H2' | 22:CA:1795:C:C6 | 2.51 | 0.46 |
| 55:DI:50:VAL:HG22 | 55:DI:85:VAL:HG13 | 1.98 | 0.46 |
| 22:CA:1982:U:OP1 | 69:CA:3704:HOH:O | 2.21 | 0.46 |
| 22:CA:749:A:H4' | 22:CA:1271:G:N3 | 2.30 | 0.46 |
| 33:CM:94:THR:CG2 | 33:CM:95:LEU:N | 2.79 | 0.46 |
| 55:DI:132:TYR:HB3 | 55:DI:133:GLU:HG2 | 1.98 | 0.46 |
| 9:BI:85:ARG:HA | 9:BI:88:MET:CE | 2.46 | 0.46 |
| 22:CA:1170:C:N4 | 22:CA:1171:G:O6 | 2.49 | 0.46 |
| 34:DN:92:TRP:HE1 | 58:DN:201:MPD:HM1 | 1.81 | 0.46 |
| 7:BG:130:ASN:ND2 | 7:BG:130:ASN:O | 2.48 | 0.46 |
| 11:BK:112:ASP:OD1 | 11:BK:114:THR:HG23 | 2.16 | 0.46 |
| 32:CL:103:VAL:O | 32:CL:122:VAL:HB | 2.16 | 0.46 |
| 30:CJ:22:PRO:HB2 | 30:CJ:23:PRO:HD3 | 1.98 | 0.46 |
| 5:AE:94:VAL:HG22 | 5:AE:111:MET:HE3 | 1.98 | 0.46 |
| 30:DJ:35:ILE:CG2 | 30:DJ:36:MET:N | 2.79 | 0.46 |
| 1:AA:872:A:C8 | 1:AA:874:G:C8 | 3.04 | 0.46 |
| 4:BD:187:GLU:N | 4:BD:190:ASP:OD2 | 2.41 | 0.46 |
| 39:CS:48:LYS:H | 39:CS:48:LYS:HE2 | 1.81 | 0.46 |
| 15:BO:26:GLU:N | 15:BO:26:GLU:OE1 | 2.44 | 0.46 |
| 44:CX:21:LEU:HA | 44:CX:39:ARG:HB2 | 1.98 | 0.46 |
| 9:BI:23:PRO:HA | 9:BI:61:LEU:HA | 1.98 | 0.46 |
| 46:DZ:11:VAL:O | 46:DZ:15:ASN:ND2 | 2.49 | 0.46 |
| 26:DE:23:PHE:CD1 | 26:DE:111:GLU:HG3 | 2.50 | 0.46 |
| 14:AN:18:ASP:OD1 | 14:AN:19:LYS:N | 2.49 | 0.46 |
| 1:BA:1108:G:H5'' | 3:BC:176:HIS:CE1 | 2.51 | 0.46 |
| 1:BA:1110:A:H8 | 1:BA:1110:A:H5' | 1.81 | 0.45 |
| 10:AJ:6:ILE:CG1 | 10:AJ:76:ILE:HB | 2.46 | 0.45 |
| 1:BA:157:U:C2' | 1:BA:158:G:H5' | 2.46 | 0.45 |
| 3:BC:64:ILE:HD13 | 3:BC:91:VAL:CG1 | 2.46 | 0.45 |
| 11:AK:111:THR:HG23 | 21:AU:3:VAL:HG22 | 1.98 | 0.45 |
| 37:DQ:2:SER:O | 37:DQ:6:LYS:HB2 | 2.16 | 0.45 |
| 1:BA:1119:C:OP2 | 9:BI:11:ARG:NH1 | 2.48 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:CE:145:ASP:HA | 26:CE:166:LYS:HB3 | 1.98 | 0.45 |
| 22:CA:483:A:H2' | 22:CA:484:C:H5' | 1.98 | 0.45 |
| 39:DS:41:ILE:HD13 | 39:DS:103:ALA:HA | 1.97 | 0.45 |
| 3:AC:77:ILE:HA | 3:AC:84:VAL:CG2 | 2.47 | 0.45 |
| 51:C4:27:ALA:O | 51:C4:28:ASN:HB2 | 2.16 | 0.45 |
| 9:BI:19:VAL:HG11 | 9:BI:83:ILE:HA | 1.98 | 0.45 |
| 8:AH:28:PRO:O | 8:AH:33:LYS:NZ | 2.38 | 0.45 |
| 24:CC:125:LYS:HB2 | 24:CC:126:PRO:HD2 | 1.98 | 0.45 |
| 11:BK:13:ARG:HG3 | 11:BK:77:TYR:HE1 | 1.80 | 0.45 |
| 53:DA:142:A:C5 | 53:DA:143:C:N4 | 2.84 | 0.45 |
| 13:BM:13:LYS:O | 13:BM:14:HIS:CG | 2.70 | 0.45 |
| 53:DA:2224:G:P | 24:DC:265:LYS:NZ | 2.89 | 0.45 |
| 14:BN:42:TRP:CD1 | 14:BN:45:VAL:HG23 | 2.51 | 0.45 |
| 53:DA:1583:A:O2' | 53:DA:1584:U:O5' | 2.30 | 0.45 |
| 1:BA:1093:A:OP1 | 7:BG:4:ARG:NH2 | 2.48 | 0.45 |
| 22:CA:2722:G:H2' | 22:CA:2723:C:C6 | 2.51 | 0.45 |
| 22:CA:2544:G:H5' | 22:CA:2645:G:C2 | 2.50 | 0.45 |
| 30:DJ:86:ILE:HD13 | 30:DJ:138:LEU:HD21 | 1.97 | 0.45 |
| 22:CA:1363:C:O2' | 22:CA:1809:A:N3 | 2.40 | 0.45 |
| 23:CB:11:C:O2' | 23:CB:15:A:N6 | 2.48 | 0.45 |
| 66:DA:3210:EDO:O1 | 57:DR:202:PG4:H32 | 2.16 | 0.45 |
| 1:BA:840:C:H2' | 1:BA:841:C:C5' | 2.46 | 0.45 |
| 1:BA:1003:G:H21 | 1:BA:1005:A:H5' | 1.81 | 0.45 |
| 22:CA:2133:G:H2' | 22:CA:2157:G:H22 | 1.82 | 0.45 |
| 41:CU:2:ILE:HG12 | 41:CU:3:ARG:N | 2.32 | 0.45 |
| 53:DA:846:U:O2' | 53:DA:847:U:P | 2.74 | 0.45 |
| 26:CE:23:PHE:CE2 | 26:CE:25:GLU:HG2 | 2.51 | 0.45 |
| 2:AB:10:LEU:HD12 | 2:AB:15:HIS:ND1 | 2.31 | 0.45 |
| 22:CA:846:U:H1' | 22:CA:847:U:C5 | 2.51 | 0.45 |
| 23:CB:14:U:H3' | 23:CB:15:A:H5' | 1.98 | 0.45 |
| 10:BJ:92:LEU:O | 10:BJ:93:ALA:HB2 | 2.16 | 0.45 |
| 37:DQ:4:ILE:H | 37:DQ:4:ILE:HD12 | 1.82 | 0.45 |
| 20:BT:5:LYS:HD3 | 20:BT:7:ALA:H | 1.80 | 0.45 |
| 7:AG:44:TYR:O | 7:AG:48:GLU:N | 2.40 | 0.45 |
| 1:AA:1170:A:H5' | 2:AB:139:ARG:NH2 | 2.30 | 0.45 |
| 27:DF:140:GLU:OE1 | 27:DF:140:GLU:N | 2.49 | 0.45 |
| 53:DA:2321:U:H5' | 53:DA:2322:A:OP2 | 2.16 | 0.45 |
| 3:AC:150:LYS:HB3 | 3:AC:169:ARG:CG | 2.46 | 0.45 |
| 22:CA:2261:C:C2 | 22:CA:2280:G:N2 | 2.84 | 0.45 |
| 53:DA:2189:U:H2' | 53:DA:2190:G:O4' | 2.16 | 0.45 |
| 22:CA:1724:G:C2' | 22:CA:1725:U:H5' | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 21:BU:21:ARG:HA | 21:BU:24:GLU:HB3 | 1.98 | 0.45 |
| 55:DI:132:TYR:H | 55:DI:133:GLU:HB2 | 1.82 | 0.45 |
| 53:DA:2886[A]:A:H2' | 53:DA:2887[A]:A:H8 | 1.81 | 0.45 |
| 22:CA:637:A:P | 33:CM:112:LEU:HB3 | 2.56 | 0.45 |
| 1:AA:657:U:O2 | 15:AO:22:THR:HG23 | 2.16 | 0.45 |
| 58:DA:3205:MPD:H52 | 58:DA:3205:MPD:HM2 | 1.98 | 0.45 |
| 22:CA:2024:G:C4 | 22:CA:2040:G:N2 | 2.84 | 0.45 |
| 22:CA:1047:G:N2 | 22:CA:1110:G:O2' | 2.50 | 0.45 |
| 1:BA:1097:C:H4' | 2:BB:139:ARG:HH21 | 1.81 | 0.45 |
| 1:AA:1423:G:OP1 | 32:DL:49:ARG:NH2 | 2.49 | 0.45 |
| 24:DC:2:ALA:N | 24:DC:20:VAL:O | 2.49 | 0.45 |
| 16:BP:2:VAL:HG13 | 16:BP:65:ALA:HA | 1.98 | 0.45 |
| 17:BQ:61:ILE:HG13 | 17:BQ:73:TRP:HE3 | 1.82 | 0.45 |
| 1:BA:833:G:C6 | 1:BA:834:U:C4 | 3.04 | 0.45 |
| 44:DX:39:ARG:HD3 | 69:DX:101:HOH:O | 2.16 | 0.45 |
| 53:DA:1171:G:C4 | 53:DA:1179:G:N2 | 2.84 | 0.45 |
| 24:CC:210:ALA:HA | 24:CC:213:TRP:NE1 | 2.32 | 0.45 |
| 53:DA:1853:A:N1 | 53:DA:2087:G:H1' | 2.31 | 0.45 |
| 55:DI:85:VAL:HG22 | 55:DI:92:ALA:HB2 | 1.98 | 0.45 |
| 22:CA:644:A:H2' | 22:CA:645:C:O4' | 2.16 | 0.45 |
| 53:DA:1539:U:H2' | 53:DA:1540:G:H8 | 1.80 | 0.45 |
| 1:BA:77:A:H2' | 1:BA:78:A:C8 | 2.52 | 0.45 |
| 13:BM:48:LEU:HD22 | 13:BM:53:ILE:HG12 | 1.99 | 0.45 |
| 1:BA:1041:G:H2' | 1:BA:1042:A:C8 | 2.51 | 0.45 |
| 55:DI:119:PRO:HG2 | 55:DI:122:GLN:HB2 | 1.98 | 0.45 |
| 22:CA:2807:U:C4 | 22:CA:2808:G:N7 | 2.84 | 0.45 |
| 1:AA:1312:G:C5' | 19:AS:6:LYS:HE2 | 2.47 | 0.45 |
| 1:BA:501:C:OP1 | 12:BL:114:ARG:NH2 | 2.50 | 0.45 |
| 22:CA:27:G:C2 | 22:CA:512:G:N3 | 2.85 | 0.45 |
| 22:CA:1906:G:C8 | 22:CA:1929:G:H2' | 2.52 | 0.45 |
| 6:BF:88:MET:SD | 6:BF:90:MET:HE2 | 2.56 | 0.45 |
| 14:BN:23:LYS:O | 14:BN:26:GLU:OE2 | 2.35 | 0.45 |
| 53:DA:1846:G:H2' | 53:DA:1847:A:C8 | 2.52 | 0.45 |
| 16:BP:46:LYS:HD3 | 16:BP:47:GLU:N | 2.26 | 0.45 |
| 1:AA:405:U:O4 | 4:AD:2:ALA:N | 2.50 | 0.45 |
| 23:CB:28:C:P | 36:CP:31:THR:HG21 | 2.57 | 0.45 |
| 1:BA:464:U:N3 | 1:BA:467:U:OP2 | 2.37 | 0.45 |
| 1:BA:1309:G:H1' | 13:BM:73:ILE:HG23 | 1.99 | 0.45 |
| 1:BA:96:U:O2' | 1:BA:97:G:H5' | 2.17 | 0.45 |
| 1:BA:542:G:H5' | 4:BD:39:GLY:HA3 | 1.98 | 0.45 |
| 5:BE:134:ILE:HD12 | 5:BE:134:ILE:H | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:DL:47:ILE:HB | 32:DL:48:PRO:HD2 | 1.98 | 0.45 |
| 7:AG:16:PRO:HB3 | 9:AI:43:THR:HG23 | 1.98 | 0.45 |
| 33:DM:81:ASP:HB3 | 33:DM:100:ILE:HD13 | 1.98 | 0.45 |
| 7:BG:26:PHE:CD2 | 7:BG:62:PHE:HE2 | 2.35 | 0.45 |
| 54:DD:85:ALA:H | 54:DD:88:GLU:HG3 | 1.82 | 0.45 |
| 5:BE:153:VAL:O | 5:BE:156:LYS:HB2 | 2.17 | 0.45 |
| 1:AA:1031:C:O2' | 1:AA:1032:G:OP2 | 2.26 | 0.45 |
| 10:AJ:67:ILE:HG13 | 14:AN:96:LEU:HD13 | 1.99 | 0.45 |
| 1:AA:1097:C:H4' | 2:AB:139:ARG:HH21 | 1.81 | 0.45 |
| 40:CT:29:VAL:CG1 | 40:CT:55:ILE:HD11 | 2.46 | 0.45 |
| 53:DA:48:G:N2 | 53:DA:49:A:N1 | 2.64 | 0.45 |
| 53:DA:836:G:OP1 | 69:DA:8111:HOH:O | 2.21 | 0.45 |
| 1:BA:1402:4OC:HM22 | 1:BA:1403:C:H5' | 1.98 | 0.45 |
| 42:CV:45:HIS:HD2 | 42:CV:58:ILE:HG23 | 1.82 | 0.45 |
| 1:AA:1079:G:H5' | 5:AE:134:ILE:CD1 | 2.46 | 0.45 |
| 21:AU:6:VAL:HG22 | 21:AU:15:ALA:HB1 | 1.99 | 0.45 |
| 1:BA:247:G:C6 | 1:BA:278:G:C2 | 3.05 | 0.45 |
| 1:AA:5:U:H6 | 1:AA:5:U:H3' | 1.81 | 0.45 |
| 29:CH:41:LYS:HA | 29:CH:44:ILE:HD13 | 1.99 | 0.45 |
| 39:CS:27:ILE:O | 39:CS:66:HIS:NE2 | 2.49 | 0.45 |
| 22:CA:2114:A:N6 | 22:CA:2119:A:N7 | 2.65 | 0.45 |
| 5:BE:148:ASN:ND2 | 5:BE:153:VAL:HG12 | 2.31 | 0.45 |
| 8:BH:7:ILE:HB | 8:BH:77:ARG:NH1 | 2.32 | 0.45 |
| 5:AE:161:VAL:O | 5:AE:164:ILE:N | 2.47 | 0.45 |
| 53:DA:2256:G:H21 | 57:DA:3193:PG4:C3 | 2.29 | 0.45 |
| 6:BF:91:ARG:HG3 | 6:BF:93:LYS:NZ | 2.32 | 0.45 |
| 35:DO:73:ASN:HA | 35:DO:76:VAL:HG13 | 1.99 | 0.45 |
| 22:CA:457:A:N1 | 22:CA:470:A:H5'' | 2.31 | 0.45 |
| 53:DA:1746:A:H2' | 53:DA:1747:U:C6 | 2.52 | 0.45 |
| 1:BA:842:U:H6 | 1:BA:842:U:O5' | 2.00 | 0.45 |
| 2:BB:124:GLY:O | 2:BB:125:THR:HG22 | 2.16 | 0.45 |
| 32:DL:113:MET:HE1 | 32:DL:116:ILE:HD11 | 1.99 | 0.45 |
| 36:DP:31:THR:HG22 | 36:DP:33:ARG:H | 1.81 | 0.45 |
| 10:AJ:5:ARG:HG2 | 10:AJ:77:VAL:HA | 1.99 | 0.45 |
| 7:BG:50:LEU:HD13 | 7:BG:61:ALA:HB1 | 1.98 | 0.45 |
| 42:CV:5:ILE:HD12 | 42:CV:67:VAL:HG12 | 1.98 | 0.45 |
| 8:AH:25:VAL:HG22 | 8:AH:63:LEU:HD21 | 1.99 | 0.45 |
| 35:DO:38:LEU:HB3 | 35:DO:39:PRO:HD3 | 1.98 | 0.45 |
| 11:BK:23:ILE:HD11 | 11:BK:93:ARG:HA | 1.98 | 0.45 |
| 62:DA:3225:SPD:C9 | 62:DA:3225:SPD:C5 | 2.94 | 0.45 |
| 22:CA:1509:A:O2' | 22:CA:1510:G:OP2 | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 7:AG:111:ARG:O | 7:AG:119:ARG:NH2 | 2.48 | 0.45 |
| 22:CA:2572:A:C8 | 25:CD:150:GLN:HB3 | 2.52 | 0.45 |
| 22:CA:1250:G:C5' | 38:CR:6:ARG:HD3 | 2.47 | 0.45 |
| 1:AA:7:A:O2' | 5:AE:106:ILE:HD11 | 2.16 | 0.45 |
| 30:CJ:18:ALA:C | 30:CJ:20:PRO:HD2 | 2.38 | 0.45 |
| 22:CA:17:G:H4' | 38:CR:25:TYR:HE2 | 1.81 | 0.45 |
| 27:CF:40:VAL:HG13 | 27:CF:41:GLY:N | 2.32 | 0.45 |
| 22:CA:2584:U:H2' | 22:CA:2585:U:H5' | 1.99 | 0.45 |
| 22:CA:193:U:H5 | 69:CA:3617:HOH:O | 1.99 | 0.45 |
| 22:CA:2303:G:H1' | 27:CF:123:ASP:HB3 | 1.99 | 0.45 |
| 34:DN:132:THR:HG22 | 34:DN:133:LYS:N | 2.32 | 0.45 |
| 1:BA:731:G:H5' | 1:BA:766:A:H4' | 1.98 | 0.45 |
| 1:AA:31:G:O2' | 1:AA:48:C:N4 | 2.50 | 0.45 |
| 16:BP:38:PHE:CE2 | 16:BP:51:ARG:HB3 | 2.52 | 0.45 |
| 51:C4:7:VAL:HB | 51:C4:61:CYS:HB3 | 1.99 | 0.45 |
| 53:DA:1932:A:H2' | 53:DA:1933:G:O4' | 2.17 | 0.45 |
| 22:CA:2291:U:H2' | 22:CA:2292:U:C6 | 2.52 | 0.45 |
| 22:CA:2046:G:H1' | 48:C1:19:HIS:CD2 | 2.52 | 0.45 |
| 38:CR:58:ARG:HG3 | 38:CR:92:ARG:HD2 | 1.98 | 0.44 |
| 1:AA:1029:U:O2' | 1:AA:1032:G:N1 | 2.49 | 0.44 |
| 25:CD:133:THR:HG23 | 25:CD:134:HIS:N | 2.32 | 0.44 |
| 50:C3:44:VAL:HG22 | 50:C3:45:SER:N | 2.32 | 0.44 |
| 22:CA:1248:G:C2 | 38:CR:3:ARG:HD2 | 2.52 | 0.44 |
| 8:BH:86:TYR:C | 8:BH:87:LYS:HD2 | 2.37 | 0.44 |
| 4:AD:58:LYS:HD2 | 4:AD:204:TYR:OH | 2.16 | 0.44 |
| 10:BJ:15:HIS:HB3 | 10:BJ:70:HIS:NE2 | 2.31 | 0.44 |
| 53:DA:629:G:H4' | 53:DA:650:C:O2 | 2.17 | 0.44 |
| 1:BA:722:G:N3 | 1:BA:722:G:H3' | 2.32 | 0.44 |
| 5:BE:50:TYR:O | 5:BE:63:ALA:HB2 | 2.17 | 0.44 |
| 53:DA:1587:G:O2' | 53:DA:1588:G:H5' | 2.17 | 0.44 |
| 53:DA:2078:C:OP1 | 69:DA:6791:HOH:O | 2.21 | 0.44 |
| 43:CW:29:ILE:HG12 | 43:CW:30:ILE:N | 2.31 | 0.44 |
| 6:BF:32:ALA:HB2 | 6:BF:70:VAL:HG11 | 1.99 | 0.44 |
| 10:AJ:52:LEU:HD23 | 10:AJ:62:ARG:HD3 | 1.97 | 0.44 |
| 2:AB:121:SER:HA | 2:AB:126:PHE:CE2 | 2.53 | 0.44 |
| 6:BF:3:HIS:CD2 | 6:BF:94:HIS:HA | 2.52 | 0.44 |
| 41:CU:17:SER:O | 41:CU:19:LYS:N | 2.38 | 0.44 |
| 7:BG:79:ARG:HG2 | 7:BG:84:THR:HA | 1.99 | 0.44 |
| 22:CA:2502:G:C5' | 22:CA:2503:2MA:H5'' | 2.47 | 0.44 |
| 41:DU:53:VAL:HG11 | 41:DU:92:ASN:HB3 | 1.99 | 0.44 |
| 2:AB:217:VAL:O | 2:AB:221:VAL:HG23 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:CA:1937:A:O2' | 22:CA:1939:5MU:H71 | 2.18 | 0.44 |
| 27:DF:132:VAL:HG22 | 27:DF:152:LEU:HB3 | 2.00 | 0.44 |
| 22:CA:543:G:H8 | 22:CA:543:G:H5'' | 1.82 | 0.44 |
| 50:C3:12:ARG:HG2 | 50:C3:12:ARG:HH21 | 1.82 | 0.44 |
| 24:CC:37:ASN:HB3 | 24:CC:60:GLN:O | 2.17 | 0.44 |
| 5:AE:74:VAL:HG22 | 5:AE:76:LEU:HD23 | 1.99 | 0.44 |
| 5:AE:105:ILE:HG23 | 5:AE:123:VAL:HG23 | 2.00 | 0.44 |
| 53:DA:57:C:H2' | 53:DA:58:G:O4' | 2.18 | 0.44 |
| 49:D2:47:VAL:CG1 | 49:D2:48:ILE:N | 2.80 | 0.44 |
| 3:AC:155:GLY:HA2 | 3:AC:163:ALA:HB1 | 2.00 | 0.44 |
| 24:CC:141:VAL:O | 24:CC:162:VAL:N | 2.43 | 0.44 |
| 35:CO:114:GLU:HB2 | 35:CO:118:ARG:HD2 | 1.99 | 0.44 |
| 1:BA:977:A:O2' | 1:BA:979:C:OP2 | 2.34 | 0.44 |
| 22:CA:2133:G:N2 | 22:CA:2158:A:C6 | 2.86 | 0.44 |
| 29:DH:116:ARG:NH2 | 29:DH:133:GLN:HB3 | 2.32 | 0.44 |
| 33:CM:100:ILE:HG12 | 33:CM:101:ILE:HG23 | 2.00 | 0.44 |
| 53:DA:2813:A:H2 | 53:DA:2887[B]:A:N6 | 2.16 | 0.44 |
| 22:CA:1581:G:C5 | 22:CA:1582:C:C5 | 3.05 | 0.44 |
| 1:AA:158:G:H2' | 1:AA:159:G:H5'' | 1.99 | 0.44 |
| 54:DD:13:ARG:HD3 | 54:DD:21:SER:OG | 2.17 | 0.44 |
| 33:CM:81:ASP:O | 33:CM:83:ALA:N | 2.50 | 0.44 |
| 35:DO:116:VAL:HG12 | 35:DO:117:ASP:N | 2.32 | 0.44 |
| 53:DA:481:G:C4 | 53:DA:507:A:C2 | 3.06 | 0.44 |
| 22:CA:247:G:H4' | 22:CA:386:G:C5 | 2.52 | 0.44 |
| 17:BQ:65:ARG:H | 17:BQ:65:ARG:HD2 | 1.83 | 0.44 |
| 22:CA:2619:C:OP1 | 25:CD:157:LYS:NZ | 2.44 | 0.44 |
| 22:CA:225:C:H2' | 22:CA:226:A:O4' | 2.17 | 0.44 |
| 22:CA:320:A:H4' | 22:CA:322:A:N7 | 2.33 | 0.44 |
| 17:AQ:8:LEU:HD13 | 17:AQ:25:ILE:HG13 | 1.99 | 0.44 |
| 5:BE:107:ALA:HB2 | 5:BE:125:ALA:HB3 | 1.99 | 0.44 |
| 20:AT:27:MET:CE | 20:AT:57:ILE:HG12 | 2.48 | 0.44 |
| 3:BC:153:VAL:HG23 | 3:BC:157:LEU:HD21 | 1.99 | 0.44 |
| 61:DA:3201:PEG:H32 | 69:DA:3916:HOH:O | 2.17 | 0.44 |
| 22:CA:449:A:OP2 | 69:CA:3239:HOH:O | 2.20 | 0.44 |
| 1:AA:1031:C:H4' | 1:AA:1032:G:O5' | 2.17 | 0.44 |
| 19:AS:29:LYS:CB | 19:AS:30:PRO:HD2 | 2.46 | 0.44 |
| 30:DJ:18:ALA:C | 30:DJ:20:PRO:HD2 | 2.37 | 0.44 |
| 53:DA:1867:G:O2' | 53:DA:1868:C:H5' | 2.17 | 0.44 |
| 20:BT:51:PHE:HA | 20:BT:54:MET:HG2 | 1.98 | 0.44 |
| 2:AB:28:LYS:N | 2:AB:29:PRO:CD | 2.81 | 0.44 |
| 41:DU:67:VAL:HG22 | 41:DU:76:ARG:HG3 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 11:AK:34:ILE:HG12 | 11:AK:70:CYS:SG | 2.58 | 0.44 |
| 53:DA:2386:A:N3 | 44:DX:41[A]:ARG:HG3 | 2.32 | 0.44 |
| 33:CM:96:LYS:HD3 | 33:CM:103:ILE:HA | 2.00 | 0.44 |
| 9:BI:50:GLN:N | 9:BI:51:PRO:HD2 | 2.33 | 0.44 |
| 3:AC:42:TYR:CZ | 3:AC:90:VAL:HG21 | 2.52 | 0.44 |
| 1:BA:977:A:H2' | 1:BA:978:A:H5'' | 2.00 | 0.44 |
| 1:BA:1219:A:OP1 | 14:BN:53:ARG:HD2 | 2.18 | 0.44 |
| 36:DP:68:LYS:CE | 61:DP:201:PEG:H41 | 2.47 | 0.44 |
| 30:DJ:20:PRO:HB2 | 30:DJ:23:PRO:CG | 2.47 | 0.44 |
| 53:DA:280:U:H2' | 53:DA:281:C:C6 | 2.53 | 0.44 |
| 1:BA:216:U:H2' | 1:BA:217:C:C6 | 2.53 | 0.44 |
| 22:CA:2349:G:OP1 | 51:C4:45:ARG:NH2 | 2.44 | 0.44 |
| 1:BA:1169:A:O2' | 2:BB:139:ARG:NH2 | 2.50 | 0.44 |
| 5:BE:24:THR:HA | 5:BE:29:ARG:HA | 1.99 | 0.44 |
| 2:BB:146:ASN:OD1 | 2:BB:146:ASN:N | 2.50 | 0.44 |
| 10:AJ:10:LEU:CD2 | 10:AJ:98:VAL:HG12 | 2.48 | 0.44 |
| 22:CA:1887:C:OP2 | 69:CA:3696:HOH:O | 2.21 | 0.44 |
| 53:DA:2628:C:H5'' | 59:DA:3195:PUT:H32 | 1.99 | 0.44 |
| 1:BA:266:G:H3' | 17:BQ:69:LYS:HB2 | 1.97 | 0.44 |
| 22:CA:674:G:H1' | 26:CE:69:ARG:CD | 2.48 | 0.44 |
| 24:CC:71:LYS:NZ | 24:CC:98:ASP:OD2 | 2.51 | 0.44 |
| 22:CA:1450:G:O6 | 22:CA:1451:C:N4 | 2.51 | 0.44 |
| 1:AA:495:A:C2 | 1:AA:496:A:C6 | 3.05 | 0.44 |
| 1:BA:1026:G:O6 | 1:BA:1035:A:N6 | 2.50 | 0.44 |
| 20:BT:67:ILE:CG1 | 20:BT:71:LYS:HD3 | 2.47 | 0.44 |
| 14:AN:30:ILE:O | 14:AN:34:VAL:HG23 | 2.17 | 0.44 |
| 53:DA:2812:G:H2' | 53:DA:2813:A:O4' | 2.18 | 0.44 |
| 3:BC:65:ARG:O | 3:BC:66:VAL:O | 2.34 | 0.44 |
| 23:CB:22:U:H2' | 23:CB:23:G:C8 | 2.52 | 0.44 |
| 11:BK:13:ARG:NH1 | 11:BK:77:TYR:OH | 2.51 | 0.44 |
| 3:AC:156:ARG:H | 3:AC:163:ALA:HA | 1.83 | 0.44 |
| 3:BC:155:GLY:HA2 | 3:BC:163:ALA:HB1 | 2.00 | 0.44 |
| 22:CA:2680:U:O2' | 22:CA:2681:C:P | 2.76 | 0.44 |
| 40:DT:110:ARG:CG | 40:DT:110:ARG:OXT | 2.66 | 0.44 |
| 53:DA:2327:A:H2' | 53:DA:2328:A:C8 | 2.52 | 0.44 |
| 9:AI:36:GLU:HA | 9:AI:45:ARG:HE | 1.83 | 0.44 |
| 1:BA:1525:G:OP1 | 11:BK:122:ARG:NH2 | 2.50 | 0.44 |
| 30:CJ:35:ILE:CG2 | 30:CJ:36:MET:N | 2.81 | 0.44 |
| 53:DA:1847:A:HO2' | 53:DA:1848:A:H8 | 1.63 | 0.44 |
| 13:AM:66:GLU:OE1 | 13:AM:70:ARG:NH2 | 2.48 | 0.44 |
| 12:AL:110:ARG:HB2 | 12:AL:119:VAL:HG21 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:AA:843:U:H3 | 2:BB:115:LYS:HD3 | 1.82 | 0.44 |
| 3:BC:40:ARG:HG2 | 3:BC:55:ILE:CG1 | 2.48 | 0.44 |
| 1:BA:1225:A:H2' | 1:BA:1226:C:C5 | 2.52 | 0.44 |
| 18:BR:34:THR:HG23 | 18:BR:36:SER:H | 1.82 | 0.44 |
| 5:AE:132:ASN:OD1 | 5:AE:134:ILE:HG22 | 2.18 | 0.44 |
| 53:DA:1783:A:H5' | 53:DA:2608:G:H4' | 1.99 | 0.44 |
| 33:DM:77:ILE:HD11 | 33:DM:101:ILE:CG2 | 2.48 | 0.44 |
| 5:BE:90:THR:HG22 | 5:BE:91:GLY:N | 2.33 | 0.44 |
| 22:CA:2307:G:N2 | 22:CA:2312:U:C4 | 2.86 | 0.44 |
| 27:DF:158:THR:CG2 | 27:DF:160:ALA:H | 2.30 | 0.44 |
| 6:BF:53:LYS:NZ | 6:BF:53:LYS:HA | 2.33 | 0.44 |
| 27:CF:103:LEU:O | 27:CF:108:VAL:HG23 | 2.17 | 0.44 |
| 53:DA:1416:G:C4 | 53:DA:1417:C:C5 | 3.06 | 0.44 |
| 22:CA:118:A:C8 | 22:CA:119:A:C8 | 3.06 | 0.44 |
| 1:AA:1463:U:H2' | 1:AA:1464:U:C6 | 2.53 | 0.44 |
| 53:DA:1721:G:H1' | 53:DA:1739:A:N6 | 2.33 | 0.44 |
| 22:CA:2582:G:C2 | 22:CA:2583:G:C8 | 3.06 | 0.44 |
| 1:AA:1322:C:P | 19:AS:78:ARG:HH22 | 2.40 | 0.44 |
| 1:AA:85:U:H6 | 1:AA:86:G:N1 | 2.15 | 0.44 |
| 17:AQ:49:GLU:O | 17:AQ:50:ASN:HB2 | 2.18 | 0.44 |
| 10:AJ:29:ALA:HA | 10:AJ:32:THR:HG22 | 2.00 | 0.44 |
| 3:AC:6:HIS:CG | 14:AN:89:MET:HB3 | 2.52 | 0.44 |
| 22:CA:12:U:H2' | 22:CA:12:U:O2 | 2.18 | 0.44 |
| 38:DR:20:GLN:HG3 | 57:DR:202:PG4:H31 | 1.98 | 0.44 |
| 22:CA:2683:C:H4' | 25:CD:13:ARG:NH1 | 2.33 | 0.44 |
| 1:BA:263:A:P | 20:BT:74:ARG:NH1 | 2.91 | 0.44 |
| 53:DA:2813:A:H2 | 53:DA:2887[B]:A:H61 | 1.63 | 0.44 |
| 22:CA:396:G:C1' | 45:CY:29:PHE:HB3 | 2.47 | 0.44 |
| 1:BA:1217:C:P | 14:BN:9:ARG:HH21 | 2.38 | 0.44 |
| 20:AT:44:LYS:HG3 | 20:AT:45:ALA:H | 1.83 | 0.44 |
| 53:DA:1494:A:C2 | 53:DA:1495:A:C4 | 3.05 | 0.44 |
| 53:DA:1494:A:HO2' | 53:DA:1495:A:P | 2.41 | 0.44 |
| 24:CC:182:ARG:NH2 | 24:CC:183:LYS:O | 2.51 | 0.44 |
| 13:BM:40:ALA:HB3 | 13:BM:43:VAL:HG13 | 2.00 | 0.44 |
| 13:BM:46:SER:O | 13:BM:47:GLU:HB3 | 2.18 | 0.44 |
| 1:AA:237:G:OP1 | 17:AQ:42:THR:OG1 | 2.30 | 0.44 |
| 3:BC:38:LYS:N | 3:BC:38:LYS:HD3 | 2.33 | 0.44 |
| 14:BN:46:LEU:HD22 | 19:BS:13:LEU:HD23 | 2.00 | 0.44 |
| 1:BA:1450:U:O2' | 1:BA:1451:U:H2' | 2.17 | 0.44 |
| 30:DJ:80:LEU:CD2 | 30:DJ:101:ILE:HD13 | 2.48 | 0.44 |
| 29:DH:31:VAL:HB | 29:DH:32:PRO:HD3 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 7:AG:72:THR:HG22 | 7:AG:142:HIS:NE2 | 2.33 | 0.44 |
| 22:CA:2030:6MZ:H9C2 | 69:CA:3585:HOH:O | 2.17 | 0.43 |
| 13:AM:4:ILE:CG2 | 13:AM:60:VAL:HG11 | 2.48 | 0.43 |
| 17:AQ:7:THR:HG21 | 17:AQ:60:GLU:CG | 2.48 | 0.43 |
| 36:CP:31:THR:HG22 | 36:CP:33:ARG:H | 1.83 | 0.43 |
| 6:BF:91:ARG:CG | 6:BF:93:LYS:NZ | 2.80 | 0.43 |
| 52:C5:1:MET:HB3 | 52:C5:34:LYS:HE2 | 2.00 | 0.43 |
| 24:DC:130:LEU:HD11 | 24:DC:135:ILE:CG1 | 2.47 | 0.43 |
| 53:DA:1539:U:C2 | 53:DA:1540:G:C8 | 3.06 | 0.43 |
| 6:BF:88:MET:SD | 6:BF:90:MET:CE | 3.06 | 0.43 |
| 2:AB:213:TYR:O | 2:AB:217:VAL:HG23 | 2.18 | 0.43 |
| 10:AJ:28:THR:O | 10:AJ:32:THR:HG22 | 2.18 | 0.43 |
| 36:DP:100:HIS:CG | 36:DP:101:GLY:N | 2.86 | 0.43 |
| 22:CA:468:G:N7 | 50:C3:39:ARG:NH2 | 2.63 | 0.43 |
| 24:DC:156:ARG:NH2 | 69:DC:393:HOH:O | 2.49 | 0.43 |
| 4:AD:188:ARG:NH2 | 4:AD:197:GLU:OE2 | 2.48 | 0.43 |
| 53:DA:1490:A:N6 | 69:DA:5107:HOH:O | 2.36 | 0.43 |
| 27:CF:33:LYS:HA | 27:CF:96:MET:SD | 2.58 | 0.43 |
| 27:CF:44:ILE:HG21 | 27:CF:79:ILE:HG22 | 2.00 | 0.43 |
| 3:AC:83:ASP:HA | 3:AC:86:LYS:HG2 | 1.99 | 0.43 |
| 41:DU:5:GLU:HG2 | 46:DZ:22:LEU:HD13 | 1.99 | 0.43 |
| 22:CA:1090:A:N1 | 22:CA:1101:U:O2 | 2.51 | 0.43 |
| 14:BN:26:GLU:N | 14:BN:26:GLU:CD | 2.61 | 0.43 |
| 1:BA:83:C:O2' | 1:BA:86:G:O6 | 2.36 | 0.43 |
| 1:BA:1127:G:H1 | 1:BA:1145:A:H61 | 1.65 | 0.43 |
| 53:DA:2161:C:H4' | 53:DA:2173:A:P | 2.58 | 0.43 |
| 8:AH:41:LYS:HD2 | 8:AH:48:ASP:HA | 2.00 | 0.43 |
| 48:C1:25:VAL:HG13 | 48:C1:26:THR:N | 2.33 | 0.43 |
| 53:DA:1187:G:H5'' | 39:DS:83:TYR:CE1 | 2.53 | 0.43 |
| 12:BL:45:PRO:HD2 | 12:BL:46:ASN:H | 1.84 | 0.43 |
| 27:CF:126:GLY:O | 27:CF:158:THR:HG21 | 2.17 | 0.43 |
| 1:AA:1014:A:OP1 | 19:AS:18:LYS:NZ | 2.51 | 0.43 |
| 53:DA:5:A:C2 | 53:DA:2899:A:C2 | 3.06 | 0.43 |
| 1:BA:993:G:O2' | 1:BA:994:A:N7 | 2.50 | 0.43 |
| 1:BA:1359:C:O2' | 1:BA:1361:G:N7 | 2.52 | 0.43 |
| 22:CA:1509:A:N3 | 22:CA:1510:G:C8 | 2.86 | 0.43 |
| 30:DJ:99:GLY:O | 30:DJ:139:VAL:HG22 | 2.17 | 0.43 |
| 61:DP:201:PEG:H42 | 61:DP:201:PEG:H22 | 1.54 | 0.43 |
| 14:AN:21:PHE:CD1 | 14:AN:55:SER:HB3 | 2.52 | 0.43 |
| 39:DS:93:PHE:HB3 | 57:DS:202:PG4:H51 | 1.99 | 0.43 |
| 5:BE:36:LEU:HD21 | 5:BE:137:VAL:HG11 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 59:DA:3195:PUT:H21 | 69:DA:5561:HOH:O | 2.18 | 0.43 |
| 2:BB:4:VAL:HG12 | 2:BB:5:SER:N | 2.33 | 0.43 |
| 29:CH:126:GLY:O | 29:CH:146:VAL:N | 2.48 | 0.43 |
| 27:DF:135:GLN:N | 27:DF:135:GLN:OE1 | 2.48 | 0.43 |
| 1:BA:268:U:H2' | 1:BA:269:C:C6 | 2.53 | 0.43 |
| 1:AA:464:U:C2 | 1:AA:466:A:H5'' | 2.53 | 0.43 |
| 10:BJ:19:ASP:HA | 10:BJ:22:THR:HB | 2.00 | 0.43 |
| 8:AH:93:PRO:HG3 | 8:AH:125:ILE:HD13 | 2.00 | 0.43 |
| 43:CW:21:ARG:NH2 | 43:CW:87:GLN:O | 2.47 | 0.43 |
| 22:CA:2578:G:OP1 | 69:CA:3833:HOH:O | 2.21 | 0.43 |
| 22:CA:2161:C:O2' | 22:CA:2173:A:OP2 | 2.36 | 0.43 |
| 5:AE:95:PHE:CZ | 5:AE:97:GLN:HG3 | 2.54 | 0.43 |
| 2:BB:121:SER:HA | 2:BB:126:PHE:CE2 | 2.53 | 0.43 |
| 2:BB:126:PHE:CG | 2:BB:127:ASP:N | 2.86 | 0.43 |
| 1:BA:532:A:H61 | 3:BC:193:TYR:HD2 | 1.66 | 0.43 |
| 53:DA:2886[A]:A:C6 | 53:DA:2887[A]:A:C5 | 3.06 | 0.43 |
| 22:CA:666:A:C5' | 33:CM:48:ARG:HD2 | 2.48 | 0.43 |
| 2:AB:27:MET:HE2 | 2:AB:189:THR:HA | 2.01 | 0.43 |
| 22:CA:1185:G:H5'' | 22:CA:1186:G:OP2 | 2.17 | 0.43 |
| 1:AA:75:G:C4 | 1:AA:76:G:C8 | 3.06 | 0.43 |
| 17:BQ:69:LYS:O | 17:BQ:71:LYS:N | 2.51 | 0.43 |
| 2:BB:32:PHE:N | 2:BB:40:ILE:O | 2.52 | 0.43 |
| 19:BS:49:ILE:HD13 | 19:BS:71:LEU:HD22 | 1.98 | 0.43 |
| 12:AL:116:LYS:NZ | 69:AL:304:HOH:O | 2.45 | 0.43 |
| 22:CA:572:A:OP2 | 39:CS:80:ARG:NH2 | 2.39 | 0.43 |
| 22:CA:125:A:OP2 | 50:C3:19:ARG:NH2 | 2.44 | 0.43 |
| 53:DA:388:G:N7 | 53:DA:390:U:H2' | 2.33 | 0.43 |
| 11:BK:106:ARG:HG2 | 11:BK:106:ARG:HH11 | 1.84 | 0.43 |
| 12:BL:51:LYS:N | 12:BL:51:LYS:HD2 | 2.33 | 0.43 |
| 22:CA:1045:C:H4' | 22:CA:1046:A:H5' | 2.00 | 0.43 |
| 14:BN:62:ASN:HB3 | 14:BN:73:PHE:CD2 | 2.53 | 0.43 |
| 22:CA:1435:G:O2' | 22:CA:1436:G:H5' | 2.19 | 0.43 |
| 22:CA:2751:G:C2 | 28:CG:3:ARG:NH1 | 2.87 | 0.43 |
| 2:AB:9:MET:CE | 2:AB:50:PHE:HD2 | 2.31 | 0.43 |
| 53:DA:1847:A:C8 | 53:DA:1847:A:P | 3.10 | 0.43 |
| 49:D2:35:GLU:OE2 | 49:D2:48:ILE:HD11 | 2.18 | 0.43 |
| 53:DA:1183:U:H2' | 53:DA:1184:U:C6 | 2.54 | 0.43 |
| 22:CA:868:U:C4 | 22:CA:869:G:N7 | 2.86 | 0.43 |
| 1:BA:1408:A:C2 | 1:BA:1494:G:C4 | 3.07 | 0.43 |
| 50:C3:24:THR:HG23 | 50:C3:27:GLY:H | 1.83 | 0.43 |
| 22:CA:782:A:H5' | 22:CA:783:A:C2 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 31:CK:57:LEU:HD23 | 31:CK:129:GLU:HA | 2.00 | 0.43 |
| 35:CO:20:MET:HG3 | 35:CO:21:PHE:N | 2.32 | 0.43 |
| 53:DA:2788:C:O2' | 53:DA:2809:A:N3 | 2.45 | 0.43 |
| 54:DD:33:ARG:NH2 | 54:DD:74:GLU:O | 2.51 | 0.43 |
| 1:BA:302:G:N3 | 1:BA:556:C:H4' | 2.34 | 0.43 |
| 22:CA:2889:C:N4 | 22:CA:2890:G:C6 | 2.87 | 0.43 |
| 53:DA:141:G:H3' | 53:DA:142:A:C4 | 2.54 | 0.43 |
| 1:BA:844:G:N3 | 1:BA:844:G:H3' | 2.33 | 0.43 |
| 11:BK:98:ARG:HG2 | 21:BU:12:PHE:HZ | 1.83 | 0.43 |
| 5:BE:44:GLY:O | 5:BE:45:ARG:O | 2.35 | 0.43 |
| 9:BI:85:ARG:HA | 9:BI:88:MET:HE3 | 2.01 | 0.43 |
| 22:CA:2716:C:O2' | 22:CA:2717:C:H5' | 2.19 | 0.43 |
| 10:AJ:56:HIS:O | 10:AJ:57:VAL:HG12 | 2.19 | 0.43 |
| 1:BA:81:A:C2 | 1:BA:89:U:O2 | 2.72 | 0.43 |
| 8:BH:29:SER:OG | 8:BH:30:SER:N | 2.51 | 0.43 |
| 55:DI:64:VAL:HG13 | 55:DI:69:PHE:HB2 | 2.01 | 0.43 |
| 9:AI:24:GLY:H | 9:AI:61:LEU:HA | 1.84 | 0.43 |
| 29:CH:23:ALA:O | 29:CH:27:ARG:N | 2.49 | 0.43 |
| 53:DA:1540:G:H2' | 53:DA:1541:C:C6 | 2.54 | 0.43 |
| 59:DA:3195:PUT:H41 | 69:DA:5231:HOH:O | 2.17 | 0.43 |
| 22:CA:55:G:C2 | 22:CA:116:C:C2 | 3.06 | 0.43 |
| 53:DA:1385:A:O2' | 53:DA:1396:U:O2 | 2.33 | 0.43 |
| 10:BJ:6:ILE:HB | 10:BJ:76:ILE:O | 2.19 | 0.43 |
| 31:CK:4:PHE:O | 38:CR:64:ARG:NH2 | 2.49 | 0.43 |
| 22:CA:2086:U:H2' | 22:CA:2087:G:C8 | 2.53 | 0.43 |
| 53:DA:876:C:H2' | 53:DA:877:A:O4' | 2.19 | 0.43 |
| 5:AE:90:THR:HG22 | 5:AE:91:GLY:N | 2.34 | 0.43 |
| 53:DA:2116:G:C6 | 53:DA:2171:A:N6 | 2.84 | 0.43 |
| 53:DA:570:G:H2' | 53:DA:2030:6MZ:N7 | 2.34 | 0.43 |
| 14:BN:49:GLN:OE1 | 19:BS:10:PHE:CZ | 2.72 | 0.43 |
| 23:CB:35:C:H2' | 23:CB:36:C:H5' | 2.00 | 0.43 |
| 30:CJ:21:SER:HB3 | 30:CJ:22:PRO:HD3 | 1.99 | 0.43 |
| 1:AA:475:C:H2' | 1:AA:476:U:O4' | 2.19 | 0.43 |
| 22:CA:2840:C:H5'' | 35:CO:53:THR:OG1 | 2.18 | 0.43 |
| 30:DJ:56:PRO:HG2 | 30:DJ:72:LYS:HB2 | 2.01 | 0.43 |
| 27:CF:50:LEU:CD2 | 27:CF:84:PRO:HB2 | 2.49 | 0.43 |
| 1:BA:1190:G:H5' | 3:BC:176:HIS:NE2 | 2.33 | 0.43 |
| 45:CY:71:LEU:HD13 | 45:CY:76:GLU:HB3 | 1.99 | 0.43 |
| 1:BA:1191:A:H5'' | 3:BC:4:LYS:HE3 | 2.01 | 0.43 |
| 1:AA:502:A:H2' | 1:AA:503:C:O4' | 2.18 | 0.43 |
| 8:AH:75:ILE:HG23 | 8:AH:75:ILE:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 53:DA:914:G:H3' | 53:DA:914:G:C8 | 2.53 | 0.43 |
| 22:CA:1871:A:O2' | 22:CA:1872:A:C8 | 2.72 | 0.43 |
| 48:D1:3:VAL:HG22 | 48:D1:4:GLN:N | 2.34 | 0.43 |
| 22:CA:1973:G:C6 | 22:CA:1974:C:C4 | 3.07 | 0.43 |
| 17:BQ:28:PHE:HD2 | 17:BQ:37:PHE:HB3 | 1.82 | 0.43 |
| 1:BA:429:U:H5' | 4:BD:9:LEU:HD12 | 2.00 | 0.43 |
| 17:BQ:49:GLU:O | 17:BQ:50:ASN:HB2 | 2.19 | 0.43 |
| 5:BE:75:ALA:O | 5:BE:82:GLN:NE2 | 2.52 | 0.43 |
| 12:BL:14:ARG:NH1 | 12:BL:15:LYS:HE2 | 2.33 | 0.43 |
| 22:CA:36:G:N3 | 22:CA:450:G:O2' | 2.51 | 0.43 |
| 1:BA:451:A:N1 | 69:BA:1879:HOH:O | 2.37 | 0.43 |
| 30:CJ:80:LEU:CD2 | 30:CJ:101:ILE:HD13 | 2.49 | 0.43 |
| 13:AM:107:ARG:HH11 | 13:AM:107:ARG:HG2 | 1.83 | 0.43 |
| 1:BA:86:G:H1' | 1:BA:87:C:C6 | 2.54 | 0.43 |
| 22:CA:335:C:HO2' | 22:CA:336:C:P | 2.41 | 0.43 |
| 1:BA:1144:G:H5" | 1:BA:1145:A:OP2 | 2.19 | 0.43 |
| 22:CA:1915:3TD:H10A | 22:CA:1916:A:C4 | 2.53 | 0.43 |
| 22:CA:1390:U:C2' | 22:CA:1391:U:H5' | 2.49 | 0.43 |
| 1:AA:1464:U:OP2 | 37:DQ:109:ARG:NH1 | 2.52 | 0.43 |
| 53:DA:1539:U:H2' | 53:DA:1540:G:C8 | 2.54 | 0.43 |
| 22:CA:2680:U:HO2' | 22:CA:2681:C:C5' | 2.32 | 0.43 |
| 24:CC:182:ARG:NH2 | 24:CC:266:PHE:HB3 | 2.34 | 0.43 |
| 29:DH:71:LYS:HB3 | 29:DH:108:VAL:HG22 | 2.00 | 0.43 |
| 22:CA:2419:U:H5" | 49:C2:22:THR:HG21 | 2.01 | 0.43 |
| 25:CD:33:ARG:NH2 | 25:CD:74:GLU:O | 2.52 | 0.43 |
| 5:BE:16:ILE:HD12 | 5:BE:16:ILE:N | 2.34 | 0.43 |
| 31:DK:69:ARG:O | 31:DK:90:GLU:HB2 | 2.19 | 0.43 |
| 11:AK:107:ILE:HG13 | 21:AU:12:PHE:CE2 | 2.54 | 0.43 |
| 22:CA:619:G:OP2 | 22:CA:620:G:N2 | 2.49 | 0.43 |
| 53:DA:1930:G:O2' | 53:DA:1931:U:OP2 | 2.37 | 0.43 |
| 1:BA:386:C:C4 | 1:BA:387:U:C5 | 3.06 | 0.43 |
| 1:BA:1498:UR3:O4' | 1:BA:1519:MA6:H2 | 2.19 | 0.43 |
| 25:CD:151:THR:C | 25:CD:153:GLY:N | 2.71 | 0.43 |
| 30:DJ:20:PRO:HB2 | 30:DJ:23:PRO:HG2 | 2.00 | 0.43 |
| 53:DA:1433:A:C2' | 53:DA:1434:A:H5' | 2.48 | 0.43 |
| 22:CA:1179:G:C5 | 22:CA:1180:U:H1' | 2.52 | 0.43 |
| 7:AG:135:VAL:HG23 | 7:AG:136:LYS:N | 2.33 | 0.43 |
| 3:BC:20:SER:OG | 3:BC:36:ASP:OD2 | 2.36 | 0.43 |
| 18:BR:72:ASP:O | 18:BR:73:ARG:HD2 | 2.19 | 0.43 |
| 9:AI:91:ASP:O | 9:AI:92:GLU:CB | 2.67 | 0.43 |
| 1:BA:209:U:H4' | 1:BA:210:C:OP2 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:AA:141:G:H2' | 1:AA:142:G:H5'' | 2.01 | 0.43 |
| 30:CJ:83:ALA:O | 30:CJ:105:GLN:NE2 | 2.51 | 0.43 |
| 53:DA:2895:G:H2' | 53:DA:2896:C:C6 | 2.54 | 0.43 |
| 24:CC:97:LYS:N | 24:CC:97:LYS:HD3 | 2.34 | 0.43 |
| 34:CN:66:ARG:NH1 | 34:CN:104:GLU:OE1 | 2.52 | 0.43 |
| 7:BG:71:PRO:HG3 | 7:BG:103:TRP:CH2 | 2.54 | 0.43 |
| 9:AI:50:GLN:N | 9:AI:51:PRO:HD2 | 2.34 | 0.43 |
| 22:CA:10:A:C2 | 22:CA:2800:A:C4 | 3.07 | 0.43 |
| 7:AG:80:VAL:HG12 | 7:AG:81:GLY:N | 2.34 | 0.43 |
| 10:BJ:26:VAL:HG13 | 10:BJ:36:VAL:HG11 | 2.01 | 0.43 |
| 46:CZ:21:LEU:CD1 | 46:CZ:46:VAL:HG13 | 2.49 | 0.43 |
| 17:BQ:74:THR:HG22 | 17:BQ:75:LEU:N | 2.34 | 0.43 |
| 50:D3:29:GLN:HG2 | 61:D3:102:PEG:H32 | 2.01 | 0.43 |
| 22:CA:319:G:C4 | 22:CA:333:G:N2 | 2.87 | 0.43 |
| 30:CJ:111:GLN:O | 30:CJ:114:ALA:HB3 | 2.19 | 0.43 |
| 30:DJ:114:ALA:CB | 30:DJ:125:MET:SD | 3.07 | 0.43 |
| 22:CA:825:A:H2' | 22:CA:826:U:O4' | 2.18 | 0.43 |
| 53:DA:1141:U:H4' | 53:DA:1142:A:O4' | 2.19 | 0.43 |
| 23:CB:35:C:O2' | 23:CB:36:C:H5' | 2.19 | 0.43 |
| 22:CA:2502:G:H5'' | 22:CA:2503:2MA:H5'' | 2.01 | 0.43 |
| 1:AA:1152:A:H5'' | 10:AJ:15:HIS:CD2 | 2.54 | 0.43 |
| 2:AB:129:LEU:O | 2:AB:130:THR:CB | 2.67 | 0.43 |
| 5:AE:94:VAL:HG13 | 5:AE:111:MET:CE | 2.49 | 0.43 |
| 22:CA:51:G:N3 | 22:CA:119:A:C2 | 2.86 | 0.43 |
| 9:AI:24:GLY:N | 9:AI:61:LEU:HA | 2.34 | 0.43 |
| 10:AJ:22:THR:HG21 | 10:AJ:39:PRO:CB | 2.49 | 0.43 |
| 22:CA:1027:A:N7 | 22:CA:1126:A:C2 | 2.86 | 0.43 |
| 1:BA:214:C:C4 | 1:BA:215:C:C5 | 3.07 | 0.43 |
| 1:AA:1328:C:H5'' | 13:AM:28:THR:HG21 | 1.99 | 0.43 |
| 13:AM:89:LEU:HD23 | 13:AM:92:ARG:HH21 | 1.84 | 0.43 |
| 31:CK:120:ARG:O | 31:CK:123:LYS:NZ | 2.49 | 0.43 |
| 33:CM:56:PRO:HB2 | 33:CM:58:TYR:CE1 | 2.54 | 0.43 |
| 5:AE:157:ARG:HD2 | 8:AH:43:GLU:O | 2.19 | 0.43 |
| 4:AD:95:GLU:OE2 | 4:AD:104:ARG:CZ | 2.67 | 0.43 |
| 53:DA:864:G:C6 | 53:DA:865:C:N4 | 2.87 | 0.43 |
| 2:AB:19:GLN:HA | 2:AB:38:VAL:HA | 2.01 | 0.43 |
| 22:CA:2632:A:C2 | 22:CA:2787:C:C2 | 3.07 | 0.43 |
| 22:CA:2478:A:OP2 | 52:C5:2:LYS:NZ | 2.51 | 0.43 |
| 5:BE:154:ALA:C | 5:BE:156:LYS:N | 2.73 | 0.42 |
| 10:AJ:53:ILE:HG22 | 10:AJ:61:ALA:O | 2.18 | 0.42 |
| 24:CC:17:VAL:HB | 24:CC:204:VAL:CG1 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:BJ:5:ARG:HH21 | 10:BJ:79:PRO:HG3 | 1.85 | 0.42 |
| 1:AA:1492:A:H2' | 1:AA:1493:A:O4' | 2.18 | 0.42 |
| 54:DD:84:LEU:HD22 | 54:DD:88:GLU:HB3 | 2.00 | 0.42 |
| 1:AA:501:C:OP1 | 12:AL:114:ARG:NH2 | 2.52 | 0.42 |
| 22:CA:2304:G:O2' | 27:CF:130:MET:O | 2.37 | 0.42 |
| 36:DP:83:LEU:HD11 | 36:DP:113:ALA:O | 2.19 | 0.42 |
| 51:C4:16:LYS:HE2 | 51:C4:20:GLY:HA2 | 2.01 | 0.42 |
| 52:C5:16:ILE:HD13 | 52:C5:25:VAL:HG22 | 2.01 | 0.42 |
| 17:BQ:15:ASP:HA | 17:BQ:21:ILE:HD12 | 2.00 | 0.42 |
| 22:CA:1790:C:O2' | 24:CC:208:ALA:HB2 | 2.18 | 0.42 |
| 17:BQ:31:HIS:HB2 | 17:BQ:38:ILE:CD1 | 2.49 | 0.42 |
| 22:CA:166:U:OP2 | 69:CA:3785:HOH:O | 2.22 | 0.42 |
| 27:DF:42:GLU:HG2 | 27:DF:49:LEU:HD23 | 2.01 | 0.42 |
| 22:CA:446:G:OP1 | 38:CR:5:LYS:NZ | 2.52 | 0.42 |
| 53:DA:2566:A:H4' | 53:DA:2567:G:H5'' | 2.01 | 0.42 |
| 22:CA:1509:A:O2' | 22:CA:1510:G:P | 2.76 | 0.42 |
| 22:CA:2032:G:N3 | 25:CD:150:GLN:HG2 | 2.33 | 0.42 |
| 22:CA:2307:G:H22 | 22:CA:2311:A:H2' | 1.84 | 0.42 |
| 14:BN:32:SER:HB2 | 14:BN:42:TRP:HE1 | 1.84 | 0.42 |
| 22:CA:1338:G:H5'' | 41:CU:17:SER:HB2 | 2.00 | 0.42 |
| 22:CA:2056:G:C2 | 22:CA:2057:G:C8 | 3.07 | 0.42 |
| 1:BA:295:C:C4 | 1:BA:296:U:C4 | 3.07 | 0.42 |
| 22:CA:1009:A:N3 | 22:CA:1153:C:O2' | 2.44 | 0.42 |
| 53:DA:1740:G:H2' | 53:DA:1741:C:O4' | 2.20 | 0.42 |
| 22:CA:1936:A:H2 | 22:CA:1943:U:H3 | 1.61 | 0.42 |
| 24:CC:121:ASP:N | 24:CC:121:ASP:OD1 | 2.51 | 0.42 |
| 43:CW:1:MET:HA | 43:CW:1:MET:CE | 2.49 | 0.42 |
| 4:BD:105:MET:SD | 4:BD:143:VAL:HG13 | 2.59 | 0.42 |
| 26:CE:75:SER:OG | 26:CE:77:ILE:HG12 | 2.18 | 0.42 |
| 2:AB:47:VAL:N | 2:AB:48:PRO:HD2 | 2.35 | 0.42 |
| 1:AA:1405:G:O4' | 1:AA:1519:MA6:H4' | 2.20 | 0.42 |
| 50:D3:33:ARG:HG2 | 61:D3:102:PEG:H42 | 2.01 | 0.42 |
| 19:BS:29:LYS:HB3 | 19:BS:30:PRO:CD | 2.49 | 0.42 |
| 22:CA:191:A:H2' | 22:CA:192:C:C6 | 2.54 | 0.42 |
| 41:CU:69:ARG:NE | 41:CU:69:ARG:O | 2.52 | 0.42 |
| 1:AA:157:U:H2' | 1:AA:158:G:H5' | 2.01 | 0.42 |
| 22:CA:846:U:H1' | 22:CA:847:U:H5 | 1.84 | 0.42 |
| 22:CA:124:G:C5 | 50:C3:19:ARG:NH1 | 2.87 | 0.42 |
| 53:DA:914:G:C3' | 53:DA:914:G:C8 | 3.02 | 0.42 |
| 26:CE:77:ILE:HG13 | 26:CE:78:TRP:HE3 | 1.84 | 0.42 |
| 22:CA:2788:C:H2' | 22:CA:2789:C:C6 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:AJ:93:ALA:HB3 | 10:AJ:96:VAL:HG23 | 2.01 | 0.42 |
| 27:DF:141:ILE:HG23 | 27:DF:146:VAL:CG1 | 2.50 | 0.42 |
| 1:BA:973:G:H1' | 10:BJ:56:HIS:HD2 | 1.84 | 0.42 |
| 1:AA:196:A:OP1 | 20:AT:64:LYS:NZ | 2.47 | 0.42 |
| 22:CA:1341:G:OP1 | 22:CA:1397:U:N3 | 2.47 | 0.42 |
| 22:CA:2531:A:H5' | 28:CG:157:TYR:CZ | 2.54 | 0.42 |
| 13:AM:32:ALA:O | 13:AM:36:ALA:N | 2.47 | 0.42 |
| 48:C1:13:ARG:HD2 | 48:C1:17:ARG:NH2 | 2.35 | 0.42 |
| 1:BA:1361:G:H2' | 1:BA:1362:A:H5' | 2.01 | 0.42 |
| 13:BM:12:HIS:O | 13:BM:13:LYS:HG3 | 2.19 | 0.42 |
| 53:DA:1172:C:N4 | 53:DA:1173:U:C2 | 2.87 | 0.42 |
| 10:AJ:65:TYR:CB | 14:AN:96:LEU:HD11 | 2.50 | 0.42 |
| 20:BT:27:MET:O | 20:BT:30:THR:OG1 | 2.31 | 0.42 |
| 32:CL:35:VAL:HG12 | 32:CL:36:GLY:N | 2.35 | 0.42 |
| 1:BA:213:G:N7 | 1:BA:214:C:C4 | 2.87 | 0.42 |
| 22:CA:830:G:C4 | 22:CA:2448:A:C5 | 3.08 | 0.42 |
| 22:CA:290:U:C2 | 22:CA:291:G:C8 | 3.07 | 0.42 |
| 22:CA:1867:G:O6 | 22:CA:1875:G:N2 | 2.52 | 0.42 |
| 22:CA:1867:G:O2' | 22:CA:1868:C:H5' | 2.19 | 0.42 |
| 11:BK:82:LEU:N | 11:BK:82:LEU:CD2 | 2.83 | 0.42 |
| 1:AA:1082:A:H2' | 1:AA:1083:U:O4' | 2.20 | 0.42 |
| 8:AH:29:SER:HB3 | 8:AH:57:PRO:HB2 | 2.00 | 0.42 |
| 1:BA:1319:A:OP2 | 19:BS:5:LEU:CD1 | 2.68 | 0.42 |
| 30:CJ:12:GLN:HA | 30:CJ:56:PRO:HA | 2.02 | 0.42 |
| 53:DA:1609:A:N6 | 69:DA:5835:HOH:O | 2.52 | 0.42 |
| 53:DA:158:U:H1' | 53:DA:169:G:N2 | 2.33 | 0.42 |
| 22:CA:634:C:H2' | 22:CA:635:C:C6 | 2.55 | 0.42 |
| 6:BF:38:ARG:NH1 | 6:BF:61:LEU:HD21 | 2.34 | 0.42 |
| 22:CA:270:A:OP1 | 22:CA:271:G:H2' | 2.20 | 0.42 |
| 53:DA:686:U:H2' | 53:DA:788:A:N1 | 2.34 | 0.42 |
| 33:CM:77:ILE:O | 33:CM:110:VAL:O | 2.37 | 0.42 |
| 2:AB:124:GLY:O | 2:AB:125:THR:HG22 | 2.19 | 0.42 |
| 35:DO:96:ARG:HD2 | 35:DO:114:GLU:OE1 | 2.19 | 0.42 |
| 1:BA:511:C:H5' | 4:BD:44:ARG:NH1 | 2.35 | 0.42 |
| 53:DA:137:U:C6 | 53:DA:140:C:C6 | 3.06 | 0.42 |
| 30:DJ:86:ILE:CD1 | 30:DJ:138:LEU:HD21 | 2.49 | 0.42 |
| 4:AD:58:LYS:HD3 | 4:AD:203:LEU:HD23 | 2.00 | 0.42 |
| 22:CA:1434:A:O2' | 22:CA:1435:G:O4' | 2.28 | 0.42 |
| 1:BA:109:A:H2' | 1:BA:326:G:N2 | 2.35 | 0.42 |
| 22:CA:1938:A:OP2 | 69:CA:3666:HOH:O | 2.21 | 0.42 |
| 22:CA:2234:G:C6 | 22:CA:2235:G:N7 | 2.87 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:CA:2143:C:H2' | 22:CA:2144:G:O4' | 2.20 | 0.42 |
| 29:DH:72:ILE:HD11 | 29:DH:110:VAL:HG21 | 2.00 | 0.42 |
| 1:AA:1431:A:C6 | 1:AA:1432:G:C6 | 3.08 | 0.42 |
| 22:CA:845:A:H3' | 22:CA:845:A:N3 | 2.35 | 0.42 |
| 22:CA:2547:A:H4' | 32:CL:29:HIS:NE2 | 2.35 | 0.42 |
| 42:DV:51:ALA:O | 42:DV:52:LEU:CB | 2.68 | 0.42 |
| 3:BC:150:LYS:HB2 | 3:BC:169:ARG:CG | 2.49 | 0.42 |
| 22:CA:41:C:H2' | 22:CA:42:A:O4' | 2.20 | 0.42 |
| 4:AD:11:LEU:O | 4:AD:15:GLU:HG2 | 2.20 | 0.42 |
| 2:BB:27:MET:CE | 2:BB:187:VAL:HG12 | 2.50 | 0.42 |
| 18:BR:20:GLU:HA | 18:BR:55:LEU:HD13 | 2.01 | 0.42 |
| 11:BK:20:VAL:N | 11:BK:35:THR:O | 2.52 | 0.42 |
| 53:DA:1482:G:H1' | 53:DA:1509:A:H61 | 1.83 | 0.42 |
| 41:CU:3:ARG:CZ | 41:CU:5:GLU:HB2 | 2.49 | 0.42 |
| 9:BI:80:ARG:O | 9:BI:84:THR:HG23 | 2.19 | 0.42 |
| 13:AM:103:LYS:HG2 | 13:AM:104:THR:HG23 | 2.01 | 0.42 |
| 14:BN:31:ILE:HG23 | 14:BN:42:TRP:CH2 | 2.55 | 0.42 |
| 30:DJ:18:ALA:O | 30:DJ:19:ASN:CB | 2.67 | 0.42 |
| 53:DA:1416:G:HO2' | 53:DA:1417:C:P | 2.42 | 0.42 |
| 3:BC:51:SER:OG | 3:BC:72:ARG:NH1 | 2.52 | 0.42 |
| 23:DB:35:C:C2' | 23:DB:36:C:H5' | 2.50 | 0.42 |
| 11:BK:17:SER:HA | 11:BK:79:ILE:HA | 2.00 | 0.42 |
| 22:CA:1638:C:H4' | 22:CA:2710:C:O2 | 2.20 | 0.42 |
| 22:CA:2020:A:H5' | 48:C1:9:THR:HG21 | 2.02 | 0.42 |
| 53:DA:1583:A:HO2' | 53:DA:1584:U:P | 2.42 | 0.42 |
| 11:BK:97:ILE:HD11 | 21:BU:16:LEU:CG | 2.50 | 0.42 |
| 42:CV:34:VAL:HG13 | 42:CV:67:VAL:HG22 | 2.02 | 0.42 |
| 22:CA:1120:G:C6 | 22:CA:1121:C:C4 | 3.07 | 0.42 |
| 1:AA:585:G:N3 | 1:AA:879:C:H4' | 2.34 | 0.42 |
| 31:CK:110:PRO:O | 31:CK:115:GLY:HA3 | 2.19 | 0.42 |
| 53:DA:382:A:C2 | 53:DA:393:C:C2 | 3.07 | 0.42 |
| 24:CC:168:ASP:N | 24:CC:168:ASP:OD1 | 2.53 | 0.42 |
| 32:CL:108:ARG:HH12 | 37:CQ:35:GLY:N | 2.17 | 0.42 |
| 22:CA:1196:C:H1' | 22:CA:1226:A:C4 | 2.54 | 0.42 |
| 3:BC:97:VAL:HB | 3:BC:98:PRO:HD2 | 2.02 | 0.42 |
| 53:DA:1405:U:H2' | 53:DA:1406:U:C6 | 2.54 | 0.42 |
| 22:CA:2636:C:H2' | 22:CA:2637:U:C6 | 2.54 | 0.42 |
| 43:DW:46:LYS:NZ | 69:DW:124:HOH:O | 2.52 | 0.42 |
| 22:CA:2824:C:C4 | 22:CA:2825:G:C5 | 3.08 | 0.42 |
| 12:AL:49:LEU:O | 12:AL:51:LYS:NZ | 2.48 | 0.42 |
| 53:DA:136:G:N1 | 53:DA:143:C:N4 | 2.65 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 41:CU:2:ILE:CG1 | 41:CU:3:ARG:N | 2.83 | 0.42 |
| 22:CA:2550:G:C5 | 22:CA:2551:C:C5 | 3.07 | 0.42 |
| 22:CA:526:A:N6 | 22:CA:2626:C:H4' | 2.34 | 0.42 |
| 22:CA:2360:G:C1' | 33:CM:60:ARG:HD3 | 2.49 | 0.42 |
| 22:CA:2189:U:H2' | 22:CA:2190:G:C5' | 2.49 | 0.42 |
| 53:DA:1868:C:H2' | 53:DA:1869:G:O4' | 2.19 | 0.42 |
| 5:BE:96:MET:CE | 5:BE:115:LEU:HD11 | 2.50 | 0.42 |
| 22:CA:1914:C:C2' | 22:CA:1915:3TD:H5'A | 2.50 | 0.42 |
| 39:CS:37:GLU:HB3 | 39:CS:53:PHE:CE1 | 2.54 | 0.42 |
| 1:BA:147:G:H2' | 1:BA:148:G:C8 | 2.54 | 0.42 |
| 53:DA:1715:G:N2 | 53:DA:1744:A:OP2 | 2.40 | 0.42 |
| 53:DA:483:A:C2' | 53:DA:484:C:H5' | 2.50 | 0.42 |
| 22:CA:289:G:H2' | 22:CA:290:U:O4' | 2.19 | 0.42 |
| 31:DK:7:LYS:O | 31:DK:11:VAL:HG23 | 2.19 | 0.42 |
| 4:BD:58:LYS:HA | 4:BD:200:ILE:HG12 | 2.01 | 0.42 |
| 1:BA:1100:C:OP2 | 2:BB:95:ARG:HD3 | 2.20 | 0.42 |
| 22:CA:2273:A:H2' | 22:CA:2274:A:C8 | 2.54 | 0.42 |
| 1:AA:1064:G:H1' | 1:AA:1190:G:N2 | 2.35 | 0.42 |
| 28:CG:101:ASN:OD1 | 28:CG:116:GLN:NE2 | 2.49 | 0.42 |
| 46:CZ:11:VAL:HG13 | 46:CZ:57:LEU:HD11 | 2.01 | 0.42 |
| 5:BE:115:LEU:HB3 | 5:BE:120:VAL:HG23 | 2.00 | 0.42 |
| 53:DA:277:G:O2' | 53:DA:278:A:OP2 | 2.37 | 0.42 |
| 22:CA:1262:A:H2 | 48:C1:7:LYS:HD2 | 1.84 | 0.42 |
| 53:DA:1132:U:H3' | 53:DA:1133:A:H5'' | 2.02 | 0.42 |
| 10:AJ:5:ARG:HH21 | 10:AJ:77:VAL:HG22 | 1.85 | 0.42 |
| 2:BB:27:MET:HE1 | 2:BB:187:VAL:O | 2.20 | 0.42 |
| 7:BG:22:LEU:HA | 7:BG:25:LYS:HE2 | 2.01 | 0.42 |
| 7:BG:145:ALA:O | 7:BG:146:GLU:CG | 2.68 | 0.42 |
| 12:AL:74:LEU:HD21 | 12:AL:104:CYS:SG | 2.60 | 0.42 |
| 40:CT:69:LEU:HB3 | 40:CT:107:VAL:HG22 | 2.00 | 0.42 |
| 1:BA:1118:U:H5'' | 9:BI:106:ARG:HG3 | 2.02 | 0.42 |
| 22:CA:933:A:H5' | 22:CA:934:U:OP2 | 2.20 | 0.42 |
| 1:BA:632:U:H2' | 1:BA:632:U:O2 | 2.20 | 0.42 |
| 53:DA:1532:A:H5'' | 53:DA:1532:A:H8 | 1.85 | 0.42 |
| 22:CA:1384:A:O2' | 22:CA:1404:C:O2 | 2.37 | 0.42 |
| 5:BE:65:GLU:OE1 | 5:BE:69:ARG:NH2 | 2.50 | 0.42 |
| 53:DA:1956:U:H2' | 53:DA:1957:C:H5' | 2.01 | 0.42 |
| 22:CA:2232:C:P | 45:CY:27:ARG:HH12 | 2.42 | 0.42 |
| 24:CC:76:ALA:HB2 | 24:CC:96:TYR:CD1 | 2.55 | 0.42 |
| 22:CA:995:C:N3 | 31:CK:3:THR:N | 2.67 | 0.42 |
| 1:AA:2:A:O2' | 4:AD:83:LYS:NZ | 2.43 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 15:BO:32:LEU:O | 15:BO:36:ILE:HG13 | 2.20 | 0.42 |
| 8:BH:78:VAL:HG11 | 8:BH:125:ILE:HD11 | 2.01 | 0.42 |
| 22:CA:820:A:C6 | 69:CA:3772:HOH:O | 2.72 | 0.42 |
| 22:CA:2127:G:N3 | 22:CA:2162:G:N7 | 2.68 | 0.42 |
| 30:CJ:99:GLY:O | 30:CJ:139:VAL:HG22 | 2.20 | 0.42 |
| 22:CA:551:G:H5' | 22:CA:551:G:H8 | 1.84 | 0.42 |
| 1:AA:1377:A:N3 | 7:AG:2:PRO:HG3 | 2.35 | 0.42 |
| 9:AI:30:ILE:HA | 9:AI:65:ILE:HG13 | 2.02 | 0.42 |
| 9:AI:19:VAL:HA | 9:AI:65:ILE:HG22 | 2.02 | 0.42 |
| 1:BA:408:A:C2 | 1:BA:435:A:C2 | 3.08 | 0.42 |
| 48:D1:41:HIS:HA | 48:D1:49:TYR:OH | 2.20 | 0.42 |
| 42:CV:86:ARG:HH12 | 42:CV:100:SER:HB3 | 1.85 | 0.42 |
| 42:CV:96:PHE:CE1 | 42:CV:103:ILE:HG13 | 2.54 | 0.42 |
| 22:CA:435:C:H2' | 22:CA:436:C:H5' | 2.00 | 0.42 |
| 22:CA:1992:G:N2 | 22:CA:1996:C:O2' | 2.53 | 0.42 |
| 3:BC:164:ARG:NH1 | 3:BC:166:GLU:OE1 | 2.53 | 0.42 |
| 53:DA:2095:A:H2' | 53:DA:2096:C:O4' | 2.20 | 0.42 |
| 22:CA:675:A:C6 | 22:CA:676:A:C6 | 3.08 | 0.42 |
| 22:CA:1352:U:OP2 | 69:CA:3353:HOH:O | 2.22 | 0.42 |
| 11:BK:31:ILE:HB | 11:BK:46:THR:HG22 | 2.02 | 0.42 |
| 1:AA:923:A:OP1 | 5:AE:26:LYS:HG2 | 2.20 | 0.42 |
| 53:DA:141:G:H2' | 53:DA:142:A:N3 | 2.33 | 0.42 |
| 27:CF:122:PHE:C | 27:CF:124:GLY:H | 2.23 | 0.42 |
| 11:AK:28:ASN:O | 11:AK:57:LYS:HD3 | 2.20 | 0.42 |
| 22:CA:335:C:H5'' | 42:CV:82:ARG:HD3 | 2.01 | 0.42 |
| 22:CA:335:C:O2' | 22:CA:336:C:P | 2.77 | 0.42 |
| 13:AM:12:HIS:HA | 13:AM:45:ILE:HG13 | 2.02 | 0.42 |
| 13:AM:33:ILE:O | 13:AM:37:ALA:N | 2.46 | 0.42 |
| 9:BI:24:GLY:N | 9:BI:61:LEU:HA | 2.35 | 0.42 |
| 53:DA:2188:U:H2' | 53:DA:2189:U:O4' | 2.19 | 0.42 |
| 3:BC:155:GLY:O | 3:BC:157:LEU:N | 2.53 | 0.42 |
| 24:CC:75:PRO:HB2 | 24:CC:97:LYS:CE | 2.50 | 0.42 |
| 10:BJ:35:GLN:HG3 | 10:BJ:36:VAL:N | 2.35 | 0.42 |
| 24:DC:247:PRO:HD2 | 24:DC:248:TRP:CE3 | 2.54 | 0.42 |
| 49:C2:48:ILE:H | 49:C2:48:ILE:HD12 | 1.84 | 0.42 |
| 3:BC:178:LEU:HD22 | 3:BC:178:LEU:H | 1.85 | 0.42 |
| 1:BA:1049:U:H2' | 14:BN:3:LYS:HE3 | 2.00 | 0.42 |
| 1:BA:1137:C:H1' | 1:BA:1138:G:N2 | 2.35 | 0.42 |
| 40:DT:1:MET:N | 40:DT:109:ASP:OD1 | 2.49 | 0.42 |
| 26:CE:42:GLY:HA3 | 26:CE:90:GLN:O | 2.19 | 0.42 |
| 5:AE:107:ALA:HB2 | 5:AE:125:ALA:HB3 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:DA:860:U:OP1 | 62:DA:3187:SPD:H92 | 2.20 | 0.42 |
| 22:CA:1272:A:C5 | 22:CA:1618:6MZ:H1' | 2.54 | 0.42 |
| 44:DX:38:VAL:HG12 | 44:DX:59:LEU:HB2 | 2.02 | 0.42 |
| 22:CA:1637:A:H5' | 22:CA:1760:C:O2' | 2.20 | 0.42 |
| 52:C5:17:VAL:CG1 | 52:C5:26:ILE:HD12 | 2.50 | 0.41 |
| 1:BA:1317:C:C2' | 14:BN:49:GLN:HE21 | 2.33 | 0.41 |
| 40:CT:84:ARG:HB2 | 40:CT:96:ILE:CD1 | 2.50 | 0.41 |
| 1:AA:1152:A:H5' | 10:AJ:72:ARG:HH22 | 1.85 | 0.41 |
| 54:DD:186:LEU:HD21 | 37:DQ:4:ILE:HG21 | 2.01 | 0.41 |
| 4:AD:95:GLU:OE2 | 4:AD:104:ARG:NH1 | 2.53 | 0.41 |
| 22:CA:2586:U:H2' | 22:CA:2587:A:O4' | 2.20 | 0.41 |
| 22:CA:214:G:HO2' | 22:CA:216:A:HO2' | 1.58 | 0.41 |
| 46:DZ:2:LYS:O | 46:DZ:3:ALA:HB3 | 2.20 | 0.41 |
| 1:BA:1213:A:O2' | 1:BA:1214:C:H5'' | 2.19 | 0.41 |
| 43:CW:24:ASN:O | 43:CW:24:ASN:ND2 | 2.53 | 0.41 |
| 58:DA:3190:MPD:C1 | 58:DA:3190:MPD:H52 | 2.50 | 0.41 |
| 53:DA:1175:A:H2' | 53:DA:1175:A:N3 | 2.35 | 0.41 |
| 40:DT:4:ILE:HG12 | 40:DT:106:VAL:HG22 | 2.02 | 0.41 |
| 31:CK:125:TYR:CE2 | 31:CK:130:HIS:HA | 2.55 | 0.41 |
| 53:DA:75:G:H4' | 46:DZ:48:ARG:NH2 | 2.35 | 0.41 |
| 53:DA:1876:A:H2' | 53:DA:1877:A:O4' | 2.20 | 0.41 |
| 18:BR:43:ARG:HG2 | 18:BR:44:ILE:H | 1.85 | 0.41 |
| 1:AA:933:G:O6 | 7:AG:3:ARG:NH1 | 2.49 | 0.41 |
| 22:CA:2615:U:C2 | 48:C1:4:GLN:HA | 2.55 | 0.41 |
| 1:BA:1001:C:H2' | 1:BA:1002:G:H8 | 1.84 | 0.41 |
| 22:CA:1059:G:H4' | 30:CJ:117:MET:HE2 | 2.02 | 0.41 |
| 32:CL:92:GLU:O | 32:CL:93:GLN:HB2 | 2.19 | 0.41 |
| 6:BF:92:THR:HG22 | 6:BF:93:LYS:N | 2.35 | 0.41 |
| 18:BR:46:GLY:O | 18:BR:47:THR:O | 2.38 | 0.41 |
| 1:BA:374:A:OP1 | 1:BA:452:A:N1 | 2.53 | 0.41 |
| 17:BQ:16:LYS:O | 17:BQ:17:MET:SD | 2.78 | 0.41 |
| 15:BO:45:GLU:HG2 | 15:BO:46:HIS:N | 2.35 | 0.41 |
| 31:DK:31:GLU:HG3 | 31:DK:142:ILE:HG13 | 2.03 | 0.41 |
| 1:AA:457:G:O6 | 1:AA:475:C:N4 | 2.45 | 0.41 |
| 24:DC:130:LEU:HD11 | 24:DC:135:ILE:HG13 | 2.02 | 0.41 |
| 22:CA:818:G:C2' | 22:CA:819:A:H5'' | 2.51 | 0.41 |
| 10:AJ:35:GLN:HB2 | 10:AJ:77:VAL:HB | 2.01 | 0.41 |
| 22:CA:674:G:H1' | 26:CE:69:ARG:NE | 2.34 | 0.41 |
| 53:DA:1084:A:C6 | 53:DA:1085:A:C6 | 3.08 | 0.41 |
| 53:DA:523:C:H4' | 53:DA:540:C:O2 | 2.20 | 0.41 |
| 21:BU:39:GLU:HG2 | 21:BU:43:THR:HB | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 53:DA:2114:A:OP2 | 53:DA:2115:G:C6 | 2.73 | 0.41 |
| 1:AA:1402:4OC:HM42 | 1:AA:1500:A:H61 | 1.85 | 0.41 |
| 22:CA:684:G:OP1 | 50:C3:16:HIS:ND1 | 2.44 | 0.41 |
| 7:AG:6:VAL:HG12 | 7:AG:7:ILE:N | 2.35 | 0.41 |
| 22:CA:2445:2MG:HM21 | 22:CA:2449:U:O4 | 2.20 | 0.41 |
| 53:DA:2129:C:N4 | 53:DA:2130:U:O4 | 2.54 | 0.41 |
| 20:AT:29:ARG:O | 20:AT:33:LYS:HG3 | 2.20 | 0.41 |
| 20:AT:28:MET:HE2 | 20:AT:32:ILE:HD11 | 2.02 | 0.41 |
| 1:AA:744:C:O2' | 1:AA:851:G:N2 | 2.48 | 0.41 |
| 53:DA:2547:A:H4' | 32:DL:29:HIS:NE2 | 2.35 | 0.41 |
| 26:CE:83:VAL:O | 26:CE:83:VAL:HG12 | 2.20 | 0.41 |
| 19:AS:63:THR:HG22 | 19:AS:65:GLU:H | 1.84 | 0.41 |
| 22:CA:250:G:P | 51:C4:13:ARG:HH12 | 2.41 | 0.41 |
| 53:DA:846:U:HO2' | 53:DA:847:U:P | 2.40 | 0.41 |
| 14:BN:53:ARG:NH2 | 19:BS:37:ARG:NH2 | 2.68 | 0.41 |
| 25:CD:104:VAL:O | 25:CD:105:LYS:HB3 | 2.20 | 0.41 |
| 1:BA:532:A:N6 | 3:BC:193:TYR:HB3 | 2.36 | 0.41 |
| 13:AM:107:ARG:NH2 | 13:AM:113:ARG:HB3 | 2.35 | 0.41 |
| 53:DA:2886[B]:A:H3' | 53:DA:2887[B]:A:C5' | 2.51 | 0.41 |
| 33:CM:111:ILE:CG2 | 33:CM:112:LEU:N | 2.83 | 0.41 |
| 54:DD:13:ARG:HD2 | 54:DD:15:PHE:CZ | 2.55 | 0.41 |
| 31:CK:80:HIS:HB3 | 31:CK:81:ILE:HG22 | 2.02 | 0.41 |
| 43:CW:21:ARG:HA | 43:CW:25:LYS:O | 2.19 | 0.41 |
| 35:CO:12:ARG:O | 35:CO:17:ARG:NH2 | 2.53 | 0.41 |
| 1:AA:757:U:O2' | 1:AA:879:C:O2 | 2.34 | 0.41 |
| 19:BS:53:ASN:ND2 | 19:BS:56:GLN:O | 2.53 | 0.41 |
| 2:BB:184:PHE:CE2 | 2:BB:198:PHE:CD1 | 3.08 | 0.41 |
| 55:DI:51:TYR:OH | 55:DI:53:ARG:NH1 | 2.53 | 0.41 |
| 24:DC:267:ILE:HD13 | 24:DC:270:ARG:HH11 | 1.85 | 0.41 |
| 26:CE:7:ASP:OD1 | 26:CE:7:ASP:N | 2.53 | 0.41 |
| 6:AF:99:ALA:HB1 | 6:AF:103:VAL:HB | 2.01 | 0.41 |
| 30:CJ:106:LEU:HD11 | 30:CJ:140:VAL:HG11 | 2.02 | 0.41 |
| 27:DF:175:PHE:HD2 | 27:DF:177:PHE:CZ | 2.38 | 0.41 |
| 34:CN:69:PRO:O | 34:CN:70:ASP:HB3 | 2.19 | 0.41 |
| 53:DA:2521:C:C2 | 53:DA:2545:G:N2 | 2.88 | 0.41 |
| 22:CA:2747:G:O6 | 22:CA:2755:C:H5'' | 2.20 | 0.41 |
| 11:AK:89:PRO:HG3 | 21:AU:32:VAL:HG11 | 2.02 | 0.41 |
| 8:BH:111:MET:HB2 | 8:BH:115:ALA:HB3 | 2.02 | 0.41 |
| 1:AA:68:G:C5 | 1:AA:69:G:H1' | 2.55 | 0.41 |
| 22:CA:279:A:H61 | 22:CA:361:G:H1' | 1.85 | 0.41 |
| 37:CQ:103:ARG:HB3 | 37:CQ:108:ALA:HB2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:BA:451:A:H5'' | 69:BP:101:HOH:O | 2.21 | 0.41 |
| 33:CM:95:LEU:HD22 | 33:CM:100:ILE:HD13 | 2.03 | 0.41 |
| 53:DA:2886[A]:A:C4 | 53:DA:2887[A]:A:C8 | 3.09 | 0.41 |
| 1:AA:842:U:H3' | 1:AA:843:U:H4' | 2.02 | 0.41 |
| 34:DN:92:TRP:NE1 | 58:DN:201:MPD:HM1 | 2.36 | 0.41 |
| 22:CA:1583:A:H1' | 22:CA:1585:C:N4 | 2.36 | 0.41 |
| 42:CV:52:LEU:HA | 42:CV:52:LEU:HD23 | 1.92 | 0.41 |
| 22:CA:1248:G:C5 | 38:CR:3:ARG:HB2 | 2.56 | 0.41 |
| 1:BA:296:U:O2' | 1:BA:556:C:O2 | 2.34 | 0.41 |
| 4:BD:105:MET:SD | 4:BD:143:VAL:CG1 | 3.09 | 0.41 |
| 1:BA:1012:A:N1 | 1:BA:1018:G:O6 | 2.53 | 0.41 |
| 53:DA:275:C:H3' | 53:DA:276:U:H5'' | 2.02 | 0.41 |
| 14:AN:54:ASP:OD1 | 14:AN:59:ARG:NE | 2.47 | 0.41 |
| 15:BO:40:GLN:HA | 15:BO:40:GLN:NE2 | 2.36 | 0.41 |
| 1:BA:421:U:H3' | 1:BA:421:U:H6 | 1.85 | 0.41 |
| 53:DA:547:A:H3' | 53:DA:547:A:C8 | 2.54 | 0.41 |
| 1:BA:254:G:H4' | 17:BQ:20:SER:HB2 | 2.01 | 0.41 |
| 25:CD:77:ARG:NH2 | 25:CD:200:ASP:OD1 | 2.44 | 0.41 |
| 22:CA:1599:U:C4 | 22:CA:1600:C:N4 | 2.89 | 0.41 |
| 53:DA:1794:A:H2' | 53:DA:1795:C:C6 | 2.55 | 0.41 |
| 1:BA:33:A:H2' | 1:BA:34:C:C6 | 2.55 | 0.41 |
| 44:CX:61:ALA:CB | 44:CX:82:ILE:HD12 | 2.50 | 0.41 |
| 1:AA:1417:G:C6 | 1:AA:1482:G:C6 | 3.08 | 0.41 |
| 28:DG:24:ILE:HD11 | 28:DG:43:VAL:HG11 | 2.02 | 0.41 |
| 1:AA:674:G:H3' | 69:AA:1910:HOH:O | 2.20 | 0.41 |
| 53:DA:141:G:C2' | 53:DA:142:A:C4 | 3.04 | 0.41 |
| 5:BE:156:LYS:O | 5:BE:159:LYS:NZ | 2.53 | 0.41 |
| 29:DH:133:GLN:HE21 | 29:DH:136:SER:HA | 1.84 | 0.41 |
| 42:CV:82:ARG:HB2 | 42:CV:97:LYS:HG3 | 2.02 | 0.41 |
| 12:BL:84:GLY:HA2 | 12:BL:95:TYR:HA | 2.02 | 0.41 |
| 10:BJ:57:VAL:HG13 | 10:BJ:58:ASN:N | 2.35 | 0.41 |
| 53:DA:435:C:C2' | 53:DA:436:C:H5' | 2.50 | 0.41 |
| 49:D2:47:VAL:HG12 | 49:D2:48:ILE:N | 2.35 | 0.41 |
| 20:BT:54:MET:HE3 | 20:BT:58:VAL:HB | 2.02 | 0.41 |
| 22:CA:11:C:H2' | 22:CA:12:U:H5' | 2.02 | 0.41 |
| 1:BA:209:U:O2 | 1:BA:209:U:H2' | 2.20 | 0.41 |
| 14:AN:62:ASN:HB3 | 14:AN:73:PHE:CD2 | 2.56 | 0.41 |
| 19:AS:40:ILE:HD11 | 19:AS:71:LEU:HD23 | 2.03 | 0.41 |
| 26:DE:87:ALA:O | 26:DE:88:ARG:HD3 | 2.21 | 0.41 |
| 29:CH:11:ASN:N | 29:CH:11:ASN:OD1 | 2.53 | 0.41 |
| 49:D2:38:LYS:NZ | 69:D2:102:HOH:O | 2.46 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:CP:15:ARG:HA | 36:CP:18:LEU:HD22 | 2.01 | 0.41 |
| 55:DI:96:PHE:O | 55:DI:100:ALA:N | 2.53 | 0.41 |
| 36:DP:16:ARG:NH2 | 69:DP:314:HOH:O | 2.42 | 0.41 |
| 22:CA:1609:A:O2' | 22:CA:1610:A:H5' | 2.21 | 0.41 |
| 33:DM:1:MET:O | 33:DM:2:ARG:HD2 | 2.20 | 0.41 |
| 53:DA:1153:C:OP2 | 69:DA:3826:HOH:O | 2.20 | 0.41 |
| 65:DA:3202:ACY:H1 | 69:DA:7057:HOH:O | 2.21 | 0.41 |
| 1:BA:977:A:C2' | 1:BA:978:A:H5'' | 2.51 | 0.41 |
| 1:BA:1255:G:C6 | 1:BA:1279:G:C8 | 3.08 | 0.41 |
| 30:DJ:117:MET:CE | 30:DJ:117:MET:HA | 2.51 | 0.41 |
| 19:BS:58:VAL:HG11 | 19:BS:75:ALA:HA | 2.02 | 0.41 |
| 2:BB:113:ARG:CZ | 2:BB:117:LEU:HD21 | 2.50 | 0.41 |
| 53:DA:1020:A:N6 | 69:DA:6936:HOH:O | 2.48 | 0.41 |
| 53:DA:1869:G:N1 | 53:DA:1873:G:C6 | 2.89 | 0.41 |
| 5:BE:133:PRO:HA | 5:BE:136:VAL:HG12 | 2.02 | 0.41 |
| 22:CA:2394:C:OP2 | 51:C4:30:ARG:HD3 | 2.21 | 0.41 |
| 22:CA:1434:A:H2' | 22:CA:1435:G:H8 | 1.85 | 0.41 |
| 14:AN:54:ASP:HA | 14:AN:59:ARG:HD3 | 2.02 | 0.41 |
| 22:CA:1833:C:C4 | 22:CA:1834:U:C4 | 3.09 | 0.41 |
| 22:CA:864:G:C6 | 22:CA:865:C:N4 | 2.89 | 0.41 |
| 8:BH:96:MET:HB3 | 8:BH:99:LEU:HB2 | 2.03 | 0.41 |
| 53:DA:2591:C:H2' | 53:DA:2592:G:C8 | 2.55 | 0.41 |
| 57:DA:3217:PG4:H32 | 57:DA:3217:PG4:H51 | 1.58 | 0.41 |
| 1:AA:510:A:H5'' | 1:AA:511:C:P | 2.61 | 0.41 |
| 22:CA:404:A:H1' | 22:CA:405:U:OP2 | 2.21 | 0.41 |
| 25:CD:1:MET:HB3 | 25:CD:205:PRO:HG2 | 2.01 | 0.41 |
| 42:CV:33:LYS:HE2 | 42:CV:66:GLN:NE2 | 2.35 | 0.41 |
| 16:AP:75:ILE:HA | 16:AP:78:VAL:HG12 | 2.01 | 0.41 |
| 15:BO:82:ILE:HG13 | 15:BO:83:GLU:N | 2.35 | 0.41 |
| 27:DF:108:VAL:HG13 | 27:DF:111:ILE:HD12 | 2.03 | 0.41 |
| 27:DF:108:VAL:N | 27:DF:109:PRO:CD | 2.84 | 0.41 |
| 1:BA:471:U:H2' | 1:BA:472:U:C6 | 2.56 | 0.41 |
| 1:BA:567:G:H2' | 1:BA:568:G:O4' | 2.19 | 0.41 |
| 11:AK:109:ASN:ND2 | 21:AU:5:LYS:HB3 | 2.36 | 0.41 |
| 53:DA:1509:A:O2' | 53:DA:1510:G:P | 2.79 | 0.41 |
| 1:BA:1361:G:H2' | 1:BA:1362:A:C5' | 2.51 | 0.41 |
| 1:AA:1224:U:H3' | 1:AA:1225:A:H5' | 2.03 | 0.41 |
| 50:C3:44:VAL:O | 50:C3:45:SER:CB | 2.69 | 0.41 |
| 22:CA:1914:C:C2 | 22:CA:1915:3TD:N1 | 2.89 | 0.41 |
| 5:AE:57:PRO:HA | 5:AE:60:ILE:CG1 | 2.51 | 0.41 |
| 31:CK:117:ALA:HA | 31:CK:120:ARG:HD2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 6:BF:38:ARG:HB3 | 6:BF:63:ASN:HB2 | 2.03 | 0.41 |
| 22:CA:42:A:C2 | 22:CA:438:G:C2 | 3.09 | 0.41 |
| 22:CA:2445:2MG:HM23 | 22:CA:2446:G:H1' | 2.02 | 0.41 |
| 2:BB:47:VAL:N | 2:BB:48:PRO:HD2 | 2.35 | 0.41 |
| 1:AA:597:G:C2 | 1:AA:644:U:C2 | 3.09 | 0.41 |
| 22:CA:7:G:H4' | 31:CK:15:TRP:CH2 | 2.56 | 0.41 |
| 41:CU:50:LEU:N | 41:CU:50:LEU:HD13 | 2.36 | 0.41 |
| 22:CA:2251:OMG:HM23 | 22:CA:2251:OMG:H1' | 1.59 | 0.41 |
| 34:CN:58:LYS:N | 34:CN:58:LYS:HD3 | 2.35 | 0.41 |
| 9:AI:54:LEU:N | 9:AI:54:LEU:HD12 | 2.36 | 0.41 |
| 24:CC:267:ILE:N | 24:CC:267:ILE:CD1 | 2.83 | 0.41 |
| 33:CM:23:ILE:H | 33:CM:23:ILE:HD12 | 1.86 | 0.41 |
| 1:AA:579:A:O2' | 15:AO:54:ARG:NH1 | 2.53 | 0.41 |
| 53:DA:2162:G:OP1 | 53:DA:2171:A:H2' | 2.20 | 0.41 |
| 53:DA:1178:C:C2' | 53:DA:1179:G:H5' | 2.51 | 0.41 |
| 9:AI:80:ARG:O | 9:AI:84:THR:HG23 | 2.20 | 0.41 |
| 5:BE:115:LEU:CA | 5:BE:120:VAL:HG23 | 2.50 | 0.41 |
| 53:DA:1417:C:H2' | 53:DA:1418:G:O4' | 2.20 | 0.41 |
| 13:BM:103:LYS:HG2 | 13:BM:104:THR:HG23 | 2.02 | 0.41 |
| 1:AA:1449:C:C2 | 1:AA:1455:G:C2 | 3.08 | 0.41 |
| 42:CV:16:GLY:O | 42:CV:18:ASP:N | 2.49 | 0.41 |
| 35:CO:116:VAL:HG12 | 35:CO:117:ASP:N | 2.35 | 0.41 |
| 19:AS:6:LYS:HD3 | 19:AS:6:LYS:HA | 1.88 | 0.41 |
| 1:AA:1079:G:H5' | 5:AE:134:ILE:HD13 | 2.03 | 0.41 |
| 5:BE:50:TYR:O | 5:BE:51:GLY:O | 2.38 | 0.41 |
| 26:CE:46:GLN:CB | 26:CE:83:VAL:HG11 | 2.51 | 0.41 |
| 53:DA:2015:A:H1' | 61:DA:3227:PEG:H42 | 2.03 | 0.41 |
| 22:CA:742:A:H2' | 22:CA:743:A:C8 | 2.55 | 0.41 |
| 22:CA:2796:U:H3 | 22:CA:2799:A:N6 | 2.19 | 0.41 |
| 22:CA:54:G:C6 | 22:CA:117:G:N2 | 2.89 | 0.41 |
| 53:DA:102:U:H2' | 53:DA:102:U:O2 | 2.20 | 0.41 |
| 35:CO:43:GLU:OE1 | 35:CO:43:GLU:HA | 2.21 | 0.41 |
| 1:AA:328:C:H2' | 1:AA:328:C:O2 | 2.21 | 0.41 |
| 29:DH:130:VAL:HG21 | 29:DH:144:VAL:HG21 | 2.02 | 0.41 |
| 25:CD:57:ALA:O | 25:CD:60:VAL:HG12 | 2.21 | 0.41 |
| 9:BI:30:ILE:HA | 9:BI:65:ILE:HG13 | 2.02 | 0.41 |
| 21:AU:4:ILE:HG23 | 21:AU:18:ARG:NH1 | 2.36 | 0.41 |
| 1:AA:1149:C:OP2 | 9:AI:11:ARG:NH2 | 2.54 | 0.41 |
| 54:DD:62:LYS:N | 54:DD:63:PRO:CD | 2.83 | 0.41 |
| 11:AK:52:PHE:O | 11:AK:53:ARG:HD2 | 2.21 | 0.41 |
| 22:CA:2032:G:C2 | 25:CD:150:GLN:HG2 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:CA:1187:G:H5'' | 39:CS:83:TYR:CE2 | 2.56 | 0.41 |
| 13:AM:6:GLY:HA2 | 13:AM:66:GLU:HG3 | 2.01 | 0.41 |
| 22:CA:1379:U:H4' | 22:CA:1380:G:OP1 | 2.21 | 0.41 |
| 12:BL:110:ARG:HB2 | 12:BL:119:VAL:HG21 | 2.03 | 0.41 |
| 5:AE:162:GLU:HG2 | 8:AH:114:ARG:NH2 | 2.36 | 0.41 |
| 15:BO:17:ARG:HD3 | 15:BO:17:ARG:H | 1.83 | 0.41 |
| 22:CA:2550:G:C6 | 22:CA:2551:C:N4 | 2.89 | 0.41 |
| 19:BS:80:TYR:CG | 19:BS:80:TYR:O | 2.74 | 0.41 |
| 22:CA:2360:G:O4' | 33:CM:60:ARG:NH2 | 2.50 | 0.41 |
| 58:DN:201:MPD:O4 | 58:DN:201:MPD:CM | 2.69 | 0.41 |
| 53:DA:355:U:H2' | 53:DA:356:G:C8 | 2.56 | 0.41 |
| 1:BA:502:A:OP1 | 12:BL:115:SER:HB3 | 2.21 | 0.41 |
| 6:BF:53:LYS:HZ2 | 6:BF:53:LYS:HA | 1.86 | 0.41 |
| 22:CA:2061:G:H5'' | 22:CA:2503:2MA:CM2 | 2.50 | 0.41 |
| 22:CA:1847:A:O2' | 22:CA:1848:A:H8 | 2.03 | 0.41 |
| 15:BO:46:HIS:O | 15:BO:48:LYS:N | 2.48 | 0.41 |
| 15:BO:87:LEU:O | 15:BO:88:ARG:CB | 2.69 | 0.41 |
| 1:BA:205:A:C2 | 1:BA:206:C:C5 | 3.08 | 0.41 |
| 7:AG:131:LYS:HA | 7:AG:135:VAL:HG21 | 2.02 | 0.41 |
| 22:CA:2271:G:H5'' | 44:CX:20:ARG:HE | 1.86 | 0.41 |
| 1:AA:1312:G:H5' | 19:AS:6:LYS:CE | 2.51 | 0.41 |
| 10:BJ:18:ILE:HD12 | 10:BJ:70:HIS:HB2 | 2.03 | 0.41 |
| 1:AA:864:A:H4' | 5:AE:90:THR:HG23 | 2.03 | 0.41 |
| 22:CA:676:A:H2 | 22:CA:2069:G7M:N3 | 2.19 | 0.41 |
| 53:DA:722:A:H2' | 53:DA:723:C:O4' | 2.20 | 0.41 |
| 49:C2:15:ALA:C | 49:C2:17:THR:H | 2.24 | 0.41 |
| 1:BA:211:G:N2 | 1:BA:212:G:H1' | 2.36 | 0.41 |
| 22:CA:2053:G:N2 | 22:CA:2054:A:H1' | 2.36 | 0.41 |
| 17:BQ:6:ARG:HB3 | 17:BQ:6:ARG:CZ | 2.51 | 0.41 |
| 1:AA:108:G:C5' | 1:AA:108:G:N3 | 2.84 | 0.41 |
| 12:BL:76:GLU:O | 12:BL:77:HIS:HB2 | 2.21 | 0.41 |
| 53:DA:118:A:C8 | 53:DA:119:A:C8 | 3.09 | 0.41 |
| 1:BA:1062:U:H2' | 1:BA:1063:C:C6 | 2.56 | 0.41 |
| 32:CL:113:MET:SD | 32:CL:116:ILE:HD11 | 2.61 | 0.41 |
| 28:CG:175:LYS:HG2 | 28:CG:176:LYS:H | 1.85 | 0.41 |
| 5:BE:13:GLU:CB | 5:BE:39:VAL:HG12 | 2.51 | 0.41 |
| 1:AA:1095:U:H2' | 1:AA:1096:C:C6 | 2.56 | 0.41 |
| 6:BF:29:ILE:HG23 | 6:BF:66:ALA:HB2 | 2.03 | 0.41 |
| 19:AS:12:ASP:OD1 | 19:AS:37:ARG:NH2 | 2.54 | 0.41 |
| 53:DA:1077:A:H4' | 30:DJ:94:ASN:HB2 | 2.03 | 0.41 |
| 53:DA:1607:C:OP1 | 69:DA:5123:HOH:O | 2.22 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 22:CA:2396:G:C2 | 22:CA:2421:G:C2 | 3.09 | 0.41 |
| 1:BA:826:C:O2 | 8:BH:16:ASN:ND2 | 2.54 | 0.41 |
| 20:AT:59:ASP:OD1 | 20:AT:76:LYS:NZ | 2.47 | 0.41 |
| 22:CA:464:U:C6 | 22:CA:788:A:C2 | 3.09 | 0.41 |
| 31:CK:41:LYS:NZ | 31:CK:50:THR:O | 2.50 | 0.41 |
| 10:BJ:87:LEU:HD13 | 10:BJ:88:MET:N | 2.35 | 0.41 |
| 3:BC:77:ILE:HA | 3:BC:84:VAL:CG2 | 2.51 | 0.41 |
| 27:CF:36:LEU:HD13 | 27:CF:36:LEU:N | 2.35 | 0.41 |
| 19:AS:31:LEU:HD12 | 19:AS:31:LEU:N | 2.36 | 0.41 |
| 20:BT:36:TYR:CD1 | 20:BT:36:TYR:C | 2.93 | 0.41 |
| 16:AP:48:GLU:HG2 | 16:AP:49:GLY:H | 1.85 | 0.41 |
| 22:CA:1693:U:O2' | 24:CC:14:ARG:NH2 | 2.54 | 0.41 |
| 49:D2:10:LYS:HE3 | 49:D2:53:LYS:O | 2.21 | 0.41 |
| 26:CE:108:ILE:HG13 | 26:CE:109:LEU:N | 2.36 | 0.41 |
| 22:CA:2650:U:O2' | 22:CA:2651:C:H5' | 2.21 | 0.41 |
| 7:BG:65:ALA:HA | 7:BG:128:ALA:HA | 2.03 | 0.41 |
| 15:BO:3:LEU:HD13 | 15:BO:35:GLN:HE21 | 1.86 | 0.41 |
| 30:CJ:113:LYS:O | 30:CJ:117:MET:HG2 | 2.21 | 0.41 |
| 1:AA:263:A:P | 20:AT:74:ARG:HH11 | 2.43 | 0.41 |
| 1:BA:1409:C:H5'' | 22:CA:1915:3TD:H10B | 2.03 | 0.41 |
| 30:CJ:20:PRO:HB2 | 30:CJ:23:PRO:HD2 | 2.03 | 0.41 |
| 53:DA:374:A:H2' | 53:DA:375:G:H5' | 2.03 | 0.41 |
| 2:AB:23:TRP:HB3 | 2:AB:39:HIS:CD2 | 2.56 | 0.41 |
| 1:AA:4:U:C2' | 1:AA:5:U:OP2 | 2.69 | 0.41 |
| 22:CA:1248:G:C4 | 38:CR:3:ARG:HD2 | 2.56 | 0.41 |
| 22:CA:2547:A:C2 | 22:CA:2562:U:C2 | 3.09 | 0.41 |
| 5:BE:39:VAL:HG22 | 5:BE:67:ALA:HB1 | 2.02 | 0.41 |
| 1:BA:106:C:O2 | 1:BA:379:C:H4' | 2.21 | 0.41 |
| 22:CA:1223:G:P | 39:CS:68:ARG:HH12 | 2.43 | 0.41 |
| 9:BI:54:LEU:N | 9:BI:54:LEU:HD12 | 2.36 | 0.41 |
| 7:BG:131:LYS:O | 7:BG:131:LYS:HG3 | 2.19 | 0.41 |
| 2:BB:138:THR:O | 2:BB:142:GLU:N | 2.44 | 0.41 |
| 1:BA:1513:A:H2' | 1:BA:1514:G:C8 | 2.56 | 0.41 |
| 33:DM:48:ARG:HD2 | 51:D4:60:ALA:O | 2.20 | 0.41 |
| 38:CR:76:TYR:CZ | 38:CR:80:ILE:HG13 | 2.56 | 0.41 |
| 15:AO:87:LEU:O | 15:AO:88:ARG:CB | 2.68 | 0.41 |
| 3:AC:85:GLU:HB2 | 3:AC:88:ARG:NH2 | 2.35 | 0.41 |
| 33:DM:78:ARG:HG2 | 33:DM:113:ALA:HB3 | 2.03 | 0.41 |
| 22:CA:2011:U:H2' | 22:CA:2012:G:O4' | 2.21 | 0.41 |
| 26:CE:131:THR:HB | 26:CE:164:LEU:HD22 | 2.02 | 0.41 |
| 14:BN:21:PHE:HB2 | 14:BN:55:SER:O | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 13:BM:13:LYS:O | 13:BM:14:HIS:ND1 | 2.55 | 0.40 |
| 66:DA:3210:EDO:O1 | 57:DR:202:PG4:C3 | 2.69 | 0.40 |
| 1:BA:1004:A:C6 | 1:BA:1005:A:C6 | 3.09 | 0.40 |
| 23:DB:90:C:H5' | 34:DN:18[A]:ARG:HG2 | 2.02 | 0.40 |
| 1:BA:1218:C:H2' | 1:BA:1219:A:C8 | 2.55 | 0.40 |
| 9:BI:95:ARG:O | 9:BI:98:LEU:N | 2.54 | 0.40 |
| 8:BH:89:LYS:HA | 8:BH:92:LEU:HG | 2.03 | 0.40 |
| 33:DM:89:VAL:O | 33:DM:94:THR:HG21 | 2.20 | 0.40 |
| 17:BQ:14:SER:C | 17:BQ:17:MET:HE1 | 2.42 | 0.40 |
| 8:AH:18:GLN:HG3 | 8:AH:70:ALA:CB | 2.52 | 0.40 |
| 9:AI:30:ILE:HB | 9:AI:65:ILE:HD11 | 2.03 | 0.40 |
| 1:BA:1053:G:P | 1:BA:1054:C:H3' | 2.61 | 0.40 |
| 53:DA:1182:G:H2' | 53:DA:1183:U:O4' | 2.22 | 0.40 |
| 1:AA:501:C:H2' | 1:AA:502:A:C8 | 2.55 | 0.40 |
| 22:CA:565:C:H2' | 22:CA:566:U:O4' | 2.21 | 0.40 |
| 22:CA:2796:U:H3 | 22:CA:2799:A:H61 | 1.68 | 0.40 |
| 1:AA:108:G:H5' | 1:AA:108:G:N3 | 2.36 | 0.40 |
| 53:DA:2389:G:H5'' | 53:DA:2390:U:O4' | 2.21 | 0.40 |
| 53:DA:1445:G:N2 | 53:DA:1547:C:C2 | 2.89 | 0.40 |
| 1:BA:75:G:C6 | 1:BA:76:G:C5 | 3.09 | 0.40 |
| 24:CC:29:PRO:HG2 | 24:CC:34:LEU:HD11 | 2.03 | 0.40 |
| 28:CG:93:GLY:HA2 | 28:CG:95:ARG:HH12 | 1.86 | 0.40 |
| 2:BB:108:ARG:HA | 2:BB:111:ILE:HG12 | 2.03 | 0.40 |
| 2:BB:118:GLU:OE2 | 2:BB:152:LYS:NZ | 2.37 | 0.40 |
| 22:CA:1857:G:O2' | 22:CA:1884:G:N2 | 2.53 | 0.40 |
| 20:BT:61:GLN:HA | 20:BT:61:GLN:OE1 | 2.21 | 0.40 |
| 5:AE:82:GLN:CD | 5:AE:150:PRO:HD3 | 2.41 | 0.40 |
| 1:AA:827:U:H5'' | 1:AA:828:U:OP2 | 2.21 | 0.40 |
| 10:BJ:27:GLU:HA | 10:BJ:30:LYS:HE2 | 2.03 | 0.40 |
| 17:BQ:58:VAL:HB | 17:BQ:79:VAL:O | 2.21 | 0.40 |
| 25:CD:2:ILE:HD13 | 25:CD:90:PHE:CZ | 2.56 | 0.40 |
| 1:BA:450:G:P | 69:BA:1918:HOH:O | 2.77 | 0.40 |
| 30:CJ:101:ILE:O | 30:CJ:141:GLU:N | 2.54 | 0.40 |
| 1:AA:841:C:C6 | 1:AA:843:U:H5' | 2.55 | 0.40 |
| 1:BA:806:C:O4' | 57:BA:1642:PG4:H72 | 2.21 | 0.40 |
| 1:BA:148:G:N3 | 1:BA:1446:A:H2 | 2.19 | 0.40 |
| 33:CM:82:LEU:HG | 33:CM:120:VAL:HG21 | 2.03 | 0.40 |
| 17:BQ:8:LEU:HD13 | 17:BQ:73:TRP:CZ3 | 2.56 | 0.40 |
| 36:CP:35:ILE:HG21 | 36:CP:71:ALA:HA | 2.03 | 0.40 |
| 22:CA:541:A:C2 | 22:CA:553:G:C2 | 3.09 | 0.40 |
| 22:CA:1468:U:H2' | 22:CA:1522:A:N6 | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 24:CC:132:MET:CE | 24:CC:172:VAL:HG21 | 2.51 | 0.40 |
| 1:BA:328:C:O2 | 1:BA:328:C:H2' | 2.21 | 0.40 |
| 26:DE:21:ARG:HD3 | 26:DE:106:LYS:HB3 | 2.03 | 0.40 |
| 62:DA:3183:SPD:H42 | 69:DA:6984:HOH:O | 2.20 | 0.40 |
| 53:DA:2650:U:O2' | 53:DA:2651:C:H5' | 2.21 | 0.40 |
| 5:BE:102:GLY:C | 5:BE:104:GLY:N | 2.70 | 0.40 |
| 25:CD:104:VAL:CG2 | 25:CD:105:LYS:N | 2.84 | 0.40 |
| 22:CA:1170:C:C2 | 22:CA:1171:G:N7 | 2.89 | 0.40 |
| 29:CH:145:ASN:HB3 | 29:CH:147:VAL:HG23 | 2.03 | 0.40 |
| 1:AA:1239:A:H62 | 1:AA:1299:A:N6 | 2.19 | 0.40 |
| 53:DA:2534:A:C2' | 53:DA:2535:G:O5' | 2.70 | 0.40 |
| 9:AI:83:ILE:HG22 | 9:AI:87:LEU:HD13 | 2.04 | 0.40 |
| 1:BA:1402:4OC:O2 | 1:BA:1402:4OC:H2' | 2.22 | 0.40 |
| 48:C1:25:VAL:HG13 | 48:C1:26:THR:H | 1.86 | 0.40 |
| 22:CA:2636:C:H4' | 25:CD:81:GLU:CD | 2.41 | 0.40 |
| 8:BH:96:MET:HB3 | 8:BH:96:MET:HE2 | 1.93 | 0.40 |
| 1:AA:579:A:H5' | 1:AA:728:A:H1' | 2.02 | 0.40 |
| 31:CK:11:VAL:HG11 | 31:CK:50:THR:HA | 2.03 | 0.40 |
| 53:DA:725:G:C6 | 53:DA:726:G:N1 | 2.90 | 0.40 |
| 53:DA:634:C:H2' | 53:DA:635:C:C6 | 2.56 | 0.40 |
| 55:DI:38:MET:O | 55:DI:41:LEU:N | 2.53 | 0.40 |
| 22:CA:310:A:H5" | 42:CV:15:THR:HG22 | 2.03 | 0.40 |
| 1:BA:1081:A:H5' | 5:BE:23:LYS:HG3 | 2.03 | 0.40 |
| 1:AA:1053:G:H5" | 1:AA:1055:A:OP1 | 2.21 | 0.40 |
| 26:CE:31:VAL:HG21 | 26:CE:104:ALA:CB | 2.51 | 0.40 |
| 22:CA:1190:G:OP1 | 33:CM:32:GLY:HA2 | 2.21 | 0.40 |
| 34:CN:20:LEU:N | 34:CN:20:LEU:HD22 | 2.35 | 0.40 |
| 24:DC:121:ASP:OD1 | 24:DC:121:ASP:N | 2.55 | 0.40 |
| 6:BF:45:ARG:O | 6:BF:56:LYS:HA | 2.21 | 0.40 |
| 27:DF:36:LEU:HD22 | 27:DF:154:ILE:HD13 | 2.03 | 0.40 |
| 1:AA:983:A:H5" | 1:AA:984:C:OP2 | 2.21 | 0.40 |
| 43:DW:2:PHE:HB3 | 43:DW:50:MET:HE1 | 2.03 | 0.40 |
| 18:BR:23:TYR:HA | 18:BR:58:ALA:HB1 | 2.03 | 0.40 |
| 38:CR:36:PHE:CE1 | 38:CR:40:ILE:HD11 | 2.56 | 0.40 |
| 1:AA:7:A:H3' | 5:AE:106:ILE:HD13 | 2.02 | 0.40 |
| 54:DD:18:ASP:HA | 57:DQ:202:PG4:H42 | 2.02 | 0.40 |
| 5:BE:81:LEU:CD1 | 5:BE:81:LEU:N | 2.84 | 0.40 |
| 22:CA:1914:C:H2' | 22:CA:1915:3TD:H5'A | 2.02 | 0.40 |
| 22:CA:662:G:O2' | 33:CM:14:LYS:HD3 | 2.22 | 0.40 |
| 1:BA:158:G:H2' | 1:BA:159:G:H5" | 2.03 | 0.40 |
| 9:BI:83:ILE:O | 9:BI:87:LEU:HD13 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:BS:13:LEU:HD22 | 19:BS:16:LEU:HD23 | 2.03 | 0.40 |
| 44:CX:34:GLY:N | 44:CX:61:ALA:O | 2.42 | 0.40 |
| 7:BG:91:VAL:O | 7:BG:96:ARG:NH2 | 2.55 | 0.40 |
| 25:CD:19:GLY:O | 32:CL:73:ASP:HB3 | 2.22 | 0.40 |
| 9:BI:124:ARG:HG3 | 9:BI:125:PRO:HD2 | 2.02 | 0.40 |
| 15:BO:10:LYS:O | 15:BO:14:GLU:HG3 | 2.21 | 0.40 |
| 22:CA:2627:G:O2' | 22:CA:2781:A:N1 | 2.41 | 0.40 |
| 53:DA:839:U:H1' | 53:DA:1191:G:H1' | 2.03 | 0.40 |
| 61:DA:3200:PEG:H32 | 61:DA:3200:PEG:H11 | 1.70 | 0.40 |
| 10:AJ:18:ILE:CG2 | 10:AJ:19:ASP:N | 2.84 | 0.40 |
| 22:CA:1651:G:H4' | 35:CO:39:PRO:HG2 | 2.03 | 0.40 |
| 32:DL:38:ILE:HD11 | 32:DL:112:PHE:HZ | 1.86 | 0.40 |
| 35:DO:33:ILE:HD11 | 48:D1:55:ILE:CD1 | 2.51 | 0.40 |
| 22:CA:2365:G:H4' | 44:CX:60:PHE:CE2 | 2.57 | 0.40 |
| 1:BA:736:C:OP1 | 18:BR:61:ARG:HD2 | 2.21 | 0.40 |
| 7:AG:113:ASP:HB2 | 7:AG:119:ARG:HG3 | 2.03 | 0.40 |
| 53:DA:1167:C:H2' | 53:DA:1168:G:H5'' | 2.04 | 0.40 |
| 1:BA:1492:A:C5 | 1:BA:1493:A:C2 | 3.10 | 0.40 |
| 14:AN:26:GLU:O | 14:AN:30:ILE:HG13 | 2.22 | 0.40 |
| 27:DF:158:THR:HG22 | 27:DF:160:ALA:N | 2.34 | 0.40 |
| 53:DA:362:A:H3' | 53:DA:363:G:H8 | 1.86 | 0.40 |
| 1:AA:1449:C:H2' | 1:AA:1450:U:H5' | 2.03 | 0.40 |
| 15:BO:67:LEU:CD2 | 15:BO:88:ARG:HH22 | 2.35 | 0.40 |
| 3:BC:11:ARG:HH21 | 3:BC:182:ILE:HG13 | 1.87 | 0.40 |
| 9:AI:57:MET:HG3 | 9:AI:61:LEU:H | 1.85 | 0.40 |
| 49:C2:50:LYS:O | 49:C2:51:GLU:HB3 | 2.22 | 0.40 |
| 9:AI:83:ILE:O | 9:AI:86:ALA:N | 2.55 | 0.40 |
| 22:CA:2680:U:H2' | 22:CA:2681:C:C6 | 2.56 | 0.40 |
| 35:CO:17:ARG:O | 35:CO:21:PHE:HD1 | 2.04 | 0.40 |
| 53:DA:1730:C:O2' | 53:DA:1731:G:O5' | 2.40 | 0.40 |
| 1:BA:706:A:H1' | 11:BK:31:ILE:HD11 | 2.04 | 0.40 |
| 53:DA:905:A:C6 | 53:DA:906:U:C5 | 3.09 | 0.40 |
| 1:BA:111:G:O6 | 1:BA:330:C:N4 | 2.55 | 0.40 |
| 53:DA:2851:A:H2' | 53:DA:2852:G:O4' | 2.22 | 0.40 |
| 22:CA:2873:A:H4' | 69:CA:3662:HOH:O | 2.22 | 0.40 |
| 43:CW:9:ARG:NH2 | 43:CW:17:SER:OG | 2.55 | 0.40 |
| 1:AA:977:A:H2' | 1:AA:978:A:H5'' | 2.04 | 0.40 |
| 2:AB:138:THR:O | 2:AB:142:GLU:N | 2.42 | 0.40 |
| 27:CF:21:ASN:ND2 | 27:CF:21:ASN:O | 2.47 | 0.40 |
| 1:BA:1111:A:H8 | 1:BA:1111:A:O5' | 2.04 | 0.40 |
| 1:AA:182:A:N1 | 1:AA:223:A:O2' | 2.53 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AA:234:C:H4' | 17:AQ:66:PRO:HG3 | 2.03 | 0.40 |
| 10:BJ:28:THR:HG23 | 10:BJ:31:ARG:NH2 | 2.36 | 0.40 |
| 1:BA:283:U:C4 | 1:BA:284:C:C4 | 3.09 | 0.40 |
| 1:AA:662:U:H2' | 1:AA:663:A:C8 | 2.56 | 0.40 |
| 22:CA:523:C:H4' | 22:CA:540:C:O2 | 2.21 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2 | AB | 222/224 (99%) | 209 (94%) | 11 (5%) | 2 (1%) | 21 | 15 |
| 2 | BB | 222/224 (99%) | 209 (94%) | 11 (5%) | 2 (1%) | 21 | 15 |
| 3 | AC | 204/206 (99%) | 193 (95%) | 10 (5%) | 1 (0%) | 34 | 30 |
| 3 | BC | 204/206 (99%) | 186 (91%) | 10 (5%) | 8 (4%) | 4 | 1 |
| 4 | AD | 203/205 (99%) | 199 (98%) | 4 (2%) | 0 | 100 | 100 |
| 4 | BD | 203/205 (99%) | 199 (98%) | 4 (2%) | 0 | 100 | 100 |
| 5 | AE | 153/155 (99%) | 145 (95%) | 8 (5%) | 0 | 100 | 100 |
| 5 | BE | 148/155 (96%) | 122 (82%) | 14 (10%) | 12 (8%) | 1 | 0 |
| 6 | AF | 104/106 (98%) | 96 (92%) | 8 (8%) | 0 | 100 | 100 |
| 6 | BF | 98/106 (92%) | 83 (85%) | 12 (12%) | 3 (3%) | 5 | 1 |
| 7 | AG | 149/151 (99%) | 138 (93%) | 10 (7%) | 1 (1%) | 26 | 21 |
| 7 | BG | 149/151 (99%) | 131 (88%) | 15 (10%) | 3 (2%) | 9 | 4 |
| 8 | AH | 127/129 (98%) | 119 (94%) | 8 (6%) | 0 | 100 | 100 |
| 8 | BH | 127/129 (98%) | 117 (92%) | 9 (7%) | 1 (1%) | 24 | 17 |
| 9 | AI | 125/127 (98%) | 111 (89%) | 13 (10%) | 1 (1%) | 24 | 17 |
| 9 | BI | 125/127 (98%) | 111 (89%) | 13 (10%) | 1 (1%) | 24 | 17 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 10 | AJ | 97/99 (98%) | 88 (91%) | 8 (8%) | 1 (1%) | 19 | 13 |
| 10 | BJ | 96/99 (97%) | 63 (66%) | 22 (23%) | 11 (12%) | 0 | 0 |
| 11 | AK | 115/117 (98%) | 104 (90%) | 11 (10%) | 0 | 100 | 100 |
| 11 | BK | 115/117 (98%) | 100 (87%) | 11 (10%) | 4 (4%) | 4 | 1 |
| 12 | AL | 120/123 (98%) | 111 (92%) | 9 (8%) | 0 | 100 | 100 |
| 12 | BL | 120/123 (98%) | 110 (92%) | 8 (7%) | 2 (2%) | 11 | 5 |
| 13 | AM | 112/114 (98%) | 101 (90%) | 8 (7%) | 3 (3%) | 6 | 2 |
| 13 | BM | 112/114 (98%) | 95 (85%) | 10 (9%) | 7 (6%) | 2 | 0 |
| 14 | AN | 98/100 (98%) | 91 (93%) | 7 (7%) | 0 | 100 | 100 |
| 14 | BN | 98/100 (98%) | 92 (94%) | 6 (6%) | 0 | 100 | 100 |
| 15 | AO | 86/88 (98%) | 80 (93%) | 3 (4%) | 3 (4%) | 4 | 1 |
| 15 | BO | 86/88 (98%) | 79 (92%) | 2 (2%) | 5 (6%) | 2 | 0 |
| 16 | AP | 80/82 (98%) | 73 (91%) | 6 (8%) | 1 (1%) | 15 | 9 |
| 16 | BP | 80/82 (98%) | 66 (82%) | 11 (14%) | 3 (4%) | 4 | 1 |
| 17 | AQ | 78/80 (98%) | 73 (94%) | 5 (6%) | 0 | 100 | 100 |
| 17 | BQ | 78/80 (98%) | 64 (82%) | 10 (13%) | 4 (5%) | 2 | 0 |
| 18 | AR | 53/55 (96%) | 51 (96%) | 1 (2%) | 1 (2%) | 10 | 4 |
| 18 | BR | 53/55 (96%) | 47 (89%) | 5 (9%) | 1 (2%) | 10 | 4 |
| 19 | AS | 77/79 (98%) | 69 (90%) | 7 (9%) | 1 (1%) | 15 | 9 |
| 19 | BS | 77/79 (98%) | 65 (84%) | 9 (12%) | 3 (4%) | 4 | 1 |
| 20 | AT | 84/86 (98%) | 83 (99%) | 1 (1%) | 0 | 100 | 100 |
| 20 | BT | 83/86 (96%) | 77 (93%) | 3 (4%) | 3 (4%) | 4 | 1 |
| 21 | AU | 54/56 (96%) | 53 (98%) | 1 (2%) | 0 | 100 | 100 |
| 21 | BU | 54/56 (96%) | 52 (96%) | 2 (4%) | 0 | 100 | 100 |
| 24 | CC | 269/271 (99%) | 251 (93%) | 15 (6%) | 3 (1%) | 17 | 11 |
| 24 | DC | 269/271 (99%) | 253 (94%) | 15 (6%) | 1 (0%) | 39 | 37 |
| 25 | CD | 207/209 (99%) | 193 (93%) | 11 (5%) | 3 (1%) | 14 | 7 |
| 26 | CE | 199/201 (99%) | 186 (94%) | 9 (4%) | 4 (2%) | 9 | 4 |
| 26 | DE | 199/201 (99%) | 195 (98%) | 4 (2%) | 0 | 100 | 100 |
| 27 | CF | 175/177 (99%) | 155 (89%) | 14 (8%) | 6 (3%) | 5 | 1 |
| 27 | DF | 175/177 (99%) | 165 (94%) | 10 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 28 | CG | 174/176 (99%) | 135 (78%) | 33 (19%) | 6 (3%) | 5 | 1 |
| 28 | DG | 174/176 (99%) | 167 (96%) | 7 (4%) | 0 | 100 | 100 |
| 29 | CH | 147/149 (99%) | 116 (79%) | 22 (15%) | 9 (6%) | 2 | 0 |
| 29 | DH | 147/149 (99%) | 129 (88%) | 16 (11%) | 2 (1%) | 14 | 7 |
| 30 | CJ | 132/134 (98%) | 117 (89%) | 11 (8%) | 4 (3%) | 5 | 2 |
| 30 | DJ | 132/134 (98%) | 117 (89%) | 11 (8%) | 4 (3%) | 5 | 2 |
| 31 | CK | 140/142 (99%) | 127 (91%) | 11 (8%) | 2 (1%) | 14 | 7 |
| 31 | DK | 140/142 (99%) | 136 (97%) | 4 (3%) | 0 | 100 | 100 |
| 32 | CL | 120/123 (98%) | 112 (93%) | 7 (6%) | 1 (1%) | 24 | 17 |
| 32 | DL | 121/123 (98%) | 116 (96%) | 4 (3%) | 1 (1%) | 24 | 17 |
| 33 | CM | 142/144 (99%) | 128 (90%) | 8 (6%) | 6 (4%) | 3 | 1 |
| 33 | DM | 142/144 (99%) | 138 (97%) | 3 (2%) | 1 (1%) | 26 | 21 |
| 34 | CN | 133/136 (98%) | 125 (94%) | 7 (5%) | 1 (1%) | 24 | 17 |
| 34 | DN | 134/136 (98%) | 128 (96%) | 6 (4%) | 0 | 100 | 100 |
| 35 | CO | 118/125 (94%) | 110 (93%) | 5 (4%) | 3 (2%) | 7 | 2 |
| 35 | DO | 123/125 (98%) | 116 (94%) | 7 (6%) | 0 | 100 | 100 |
| 36 | CP | 114/117 (97%) | 105 (92%) | 4 (4%) | 5 (4%) | 3 | 1 |
| 36 | DP | 115/117 (98%) | 112 (97%) | 3 (3%) | 0 | 100 | 100 |
| 37 | CQ | 112/114 (98%) | 104 (93%) | 7 (6%) | 1 (1%) | 21 | 15 |
| 37 | DQ | 112/114 (98%) | 107 (96%) | 5 (4%) | 0 | 100 | 100 |
| 38 | CR | 115/117 (98%) | 114 (99%) | 1 (1%) | 0 | 100 | 100 |
| 38 | DR | 115/117 (98%) | 114 (99%) | 1 (1%) | 0 | 100 | 100 |
| 39 | CS | 101/103 (98%) | 93 (92%) | 5 (5%) | 3 (3%) | 5 | 2 |
| 39 | DS | 101/103 (98%) | 98 (97%) | 3 (3%) | 0 | 100 | 100 |
| 40 | CT | 108/110 (98%) | 101 (94%) | 4 (4%) | 3 (3%) | 6 | 2 |
| 40 | DT | 108/110 (98%) | 105 (97%) | 3 (3%) | 0 | 100 | 100 |
| 41 | CU | 91/93 (98%) | 81 (89%) | 7 (8%) | 3 (3%) | 5 | 1 |
| 41 | DU | 91/93 (98%) | 83 (91%) | 7 (8%) | 1 (1%) | 17 | 11 |
| 42 | CV | 100/102 (98%) | 81 (81%) | 11 (11%) | 8 (8%) | 1 | 0 |
| 42 | DV | 100/102 (98%) | 96 (96%) | 3 (3%) | 1 (1%) | 19 | 13 |
| 43 | CW | 92/94 (98%) | 86 (94%) | 6 (6%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 43 | DW | 92/94 (98%) | 87 (95%) | 5 (5%) | 0 | 100 | 100 |
| 44 | CX | 73/76 (96%) | 72 (99%) | 1 (1%) | 0 | 100 | 100 |
| 44 | DX | 75/76 (99%) | 74 (99%) | 1 (1%) | 0 | 100 | 100 |
| 45 | CY | 75/77 (97%) | 72 (96%) | 3 (4%) | 0 | 100 | 100 |
| 45 | DY | 75/77 (97%) | 72 (96%) | 3 (4%) | 0 | 100 | 100 |
| 46 | CZ | 60/62 (97%) | 52 (87%) | 5 (8%) | 3 (5%) | 3 | 0 |
| 46 | DZ | 60/62 (97%) | 59 (98%) | 1 (2%) | 0 | 100 | 100 |
| 47 | C0 | 56/58 (97%) | 51 (91%) | 4 (7%) | 1 (2%) | 11 | 5 |
| 47 | D0 | 57/58 (98%) | 54 (95%) | 2 (4%) | 1 (2%) | 11 | 5 |
| 48 | C1 | 54/56 (96%) | 48 (89%) | 4 (7%) | 2 (4%) | 4 | 1 |
| 48 | D1 | 54/56 (96%) | 52 (96%) | 2 (4%) | 0 | 100 | 100 |
| 49 | C2 | 48/51 (94%) | 41 (85%) | 6 (12%) | 1 (2%) | 9 | 3 |
| 49 | D2 | 49/51 (96%) | 47 (96%) | 2 (4%) | 0 | 100 | 100 |
| 50 | C3 | 44/46 (96%) | 40 (91%) | 2 (4%) | 2 (4%) | 3 | 1 |
| 50 | D3 | 44/46 (96%) | 43 (98%) | 1 (2%) | 0 | 100 | 100 |
| 51 | C4 | 62/64 (97%) | 59 (95%) | 3 (5%) | 0 | 100 | 100 |
| 51 | D4 | 62/64 (97%) | 59 (95%) | 3 (5%) | 0 | 100 | 100 |
| 52 | C5 | 36/38 (95%) | 34 (94%) | 2 (6%) | 0 | 100 | 100 |
| 52 | D5 | 36/38 (95%) | 35 (97%) | 1 (3%) | 0 | 100 | 100 |
| 54 | DD | 206/209 (99%) | 199 (97%) | 7 (3%) | 0 | 100 | 100 |
| 55 | DI | 133/135 (98%) | 107 (80%) | 19 (14%) | 7 (5%) | 2 | 0 |
| All | All | 11407/11629 (98%) | 10507 (92%) | 713 (6%) | 187 (2%) | 12 | 6 |

All (187) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 130 | THR |
| 3 | AC | 127 | ARG |
| 9 | AI | 25 | ASN |
| 10 | AJ | 57 | VAL |
| 13 | AM | 5 | ALA |
| 2 | BB | 130 | THR |
| 3 | BC | 66 | VAL |
| 3 | BC | 127 | ARG |
| 3 | BC | 139 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | BC | 140 | ASN |
| 5 | BE | 24 | THR |
| 5 | BE | 45 | ARG |
| 5 | BE | 51 | GLY |
| 5 | BE | 102 | GLY |
| 5 | BE | 103 | THR |
| 5 | BE | 123 | VAL |
| 6 | BF | 53 | LYS |
| 6 | BF | 98 | GLU |
| 9 | BI | 25 | ASN |
| 10 | BJ | 93 | ALA |
| 11 | BK | 52 | PHE |
| 12 | BL | 44 | LYS |
| 13 | BM | 5 | ALA |
| 13 | BM | 14 | HIS |
| 16 | BP | 43 | ALA |
| 16 | BP | 79 | ASN |
| 16 | BP | 80 | LYS |
| 17 | BQ | 17 | MET |
| 18 | BR | 47 | THR |
| 19 | BS | 5 | LEU |
| 25 | CD | 152 | PRO |
| 26 | CE | 42 | GLY |
| 26 | CE | 153 | LEU |
| 27 | CF | 62 | GLY |
| 27 | CF | 123 | ASP |
| 28 | CG | 119 | ALA |
| 29 | CH | 3 | VAL |
| 29 | CH | 9 | VAL |
| 29 | CH | 10 | ALA |
| 29 | CH | 137 | GLU |
| 30 | CJ | 15 | ALA |
| 30 | CJ | 19 | ASN |
| 31 | CK | 81 | ILE |
| 33 | CM | 82 | LEU |
| 33 | CM | 86 | GLU |
| 33 | CM | 111 | ILE |
| 35 | CO | 70 | THR |
| 36 | CP | 59 | ALA |
| 37 | CQ | 114 | LEU |
| 40 | CT | 65 | ASP |
| 41 | CU | 17 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42 | CV | 7 | ARG |
| 46 | CZ | 3 | ALA |
| 48 | C1 | 56 | ALA |
| 50 | C3 | 44 | VAL |
| 55 | DI | 67 | THR |
| 55 | DI | 104 | ALA |
| 55 | DI | 106 | PHE |
| 30 | DJ | 15 | ALA |
| 30 | DJ | 19 | ASN |
| 42 | DV | 52 | LEU |
| 13 | AM | 13 | LYS |
| 15 | AO | 88 | ARG |
| 3 | BC | 81 | GLY |
| 3 | BC | 141 | ALA |
| 3 | BC | 156 | ARG |
| 5 | BE | 111 | MET |
| 5 | BE | 155 | ALA |
| 5 | BE | 157 | ARG |
| 6 | BF | 52 | ASN |
| 7 | BG | 146 | GLU |
| 8 | BH | 89 | LYS |
| 10 | BJ | 17 | LEU |
| 10 | BJ | 41 | PRO |
| 10 | BJ | 57 | VAL |
| 10 | BJ | 89 | ARG |
| 10 | BJ | 90 | LEU |
| 11 | BK | 89 | PRO |
| 11 | BK | 93 | ARG |
| 13 | BM | 4 | ILE |
| 13 | BM | 67 | GLY |
| 15 | BO | 88 | ARG |
| 17 | BQ | 70 | THR |
| 19 | BS | 6 | LYS |
| 20 | BT | 68 | HIS |
| 24 | CC | 253 | LYS |
| 25 | CD | 104 | VAL |
| 26 | CE | 82 | GLY |
| 27 | CF | 121 | SER |
| 27 | CF | 149 | VAL |
| 28 | CG | 92 | VAL |
| 28 | CG | 175 | LYS |
| 29 | CH | 16 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30 | CJ | 25 | GLY |
| 31 | CK | 25 | LEU |
| 32 | CL | 35 | VAL |
| 33 | CM | 30 | THR |
| 35 | CO | 119 | SER |
| 36 | CP | 101 | GLY |
| 39 | CS | 29 | THR |
| 40 | CT | 62 | ASP |
| 40 | CT | 63 | GLY |
| 41 | CU | 18 | GLU |
| 41 | CU | 38 | ALA |
| 42 | CV | 19 | LYS |
| 42 | CV | 52 | LEU |
| 42 | CV | 75 | ALA |
| 42 | CV | 99 | ASN |
| 50 | C3 | 45 | SER |
| 24 | DC | 253 | LYS |
| 29 | DH | 118 | PRO |
| 55 | DI | 108 | VAL |
| 30 | DJ | 25 | GLY |
| 32 | DL | 108 | ARG |
| 2 | AB | 126 | PHE |
| 16 | AP | 48 | GLU |
| 18 | AR | 73 | ARG |
| 5 | BE | 138 | ARG |
| 10 | BJ | 43 | PRO |
| 10 | BJ | 95 | GLY |
| 11 | BK | 92 | GLY |
| 13 | BM | 114 | LYS |
| 15 | BO | 18 | ASP |
| 15 | BO | 46 | HIS |
| 15 | BO | 47 | LYS |
| 25 | CD | 86 | GLU |
| 28 | CG | 118 | PRO |
| 29 | CH | 2 | GLN |
| 29 | CH | 118 | PRO |
| 30 | CJ | 23 | PRO |
| 33 | CM | 29 | LYS |
| 33 | CM | 115 | GLU |
| 34 | CN | 69 | PRO |
| 36 | CP | 57 | ALA |
| 36 | CP | 66 | GLY |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 39 | CS | 53 | PHE |
| 42 | CV | 55 | PRO |
| 42 | CV | 98 | SER |
| 46 | CZ | 37 | LEU |
| 47 | C0 | 4 | THR |
| 55 | DI | 124 | ASP |
| 30 | DJ | 23 | PRO |
| 47 | D0 | 4 | THR |
| 7 | AG | 80 | VAL |
| 15 | AO | 18 | ASP |
| 15 | AO | 21 | ASP |
| 2 | BB | 126 | PHE |
| 3 | BC | 80 | LYS |
| 10 | BJ | 36 | VAL |
| 10 | BJ | 101 | SER |
| 27 | CF | 174 | ASP |
| 27 | CF | 175 | PHE |
| 29 | CH | 33 | GLN |
| 35 | CO | 118 | ARG |
| 36 | CP | 100 | HIS |
| 48 | C1 | 55 | ILE |
| 55 | DI | 130 | PRO |
| 13 | AM | 105 | ASN |
| 5 | BE | 12 | GLN |
| 7 | BG | 80 | VAL |
| 7 | BG | 82 | GLY |
| 15 | BO | 21 | ASP |
| 17 | BQ | 18 | GLU |
| 28 | CG | 59 | ALA |
| 29 | CH | 31 | VAL |
| 49 | C2 | 16 | GLY |
| 55 | DI | 68 | PRO |
| 33 | DM | 29 | LYS |
| 19 | AS | 29 | LYS |
| 10 | BJ | 34 | ALA |
| 13 | BM | 13 | LYS |
| 17 | BQ | 82 | ALA |
| 20 | BT | 4 | ILE |
| 20 | BT | 5 | LYS |
| 24 | CC | 261 | LYS |
| 42 | CV | 56 | GLY |
| 29 | DH | 122 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | BS | 29 | LYS |
| 28 | CG | 28 | GLY |
| 24 | CC | 3 | VAL |
| 12 | BL | 45 | PRO |
| 13 | BM | 7 | ILE |
| 39 | CS | 50 | GLY |
| 46 | CZ | 46 | VAL |
| 5 | BE | 137 | VAL |
| 26 | CE | 83 | VAL |
| 41 | DU | 90 | GLY |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2 | AB | 186/186 (100%) | 180 (97%) | 6 (3%) | 46 | 48 |
| 2 | BB | 186/186 (100%) | 179 (96%) | 7 (4%) | 40 | 40 |
| 3 | AC | 170/170 (100%) | 164 (96%) | 6 (4%) | 43 | 44 |
| 3 | BC | 170/170 (100%) | 142 (84%) | 28 (16%) | 3 | 1 |
| 4 | AD | 172/172 (100%) | 167 (97%) | 5 (3%) | 50 | 53 |
| 4 | BD | 172/172 (100%) | 167 (97%) | 5 (3%) | 50 | 53 |
| 5 | AE | 118/118 (100%) | 112 (95%) | 6 (5%) | 29 | 26 |
| 5 | BE | 113/118 (96%) | 92 (81%) | 21 (19%) | 2 | 1 |
| 6 | AF | 92/92 (100%) | 91 (99%) | 1 (1%) | 80 | 85 |
| 6 | BF | 87/92 (95%) | 73 (84%) | 14 (16%) | 3 | 1 |
| 7 | AG | 124/124 (100%) | 121 (98%) | 3 (2%) | 57 | 61 |
| 7 | BG | 124/124 (100%) | 97 (78%) | 27 (22%) | 1 | 0 |
| 8 | AH | 104/104 (100%) | 100 (96%) | 4 (4%) | 40 | 40 |
| 8 | BH | 104/104 (100%) | 87 (84%) | 17 (16%) | 3 | 1 |
| 9 | AI | 105/105 (100%) | 102 (97%) | 3 (3%) | 50 | 53 |
| 9 | BI | 105/105 (100%) | 102 (97%) | 3 (3%) | 50 | 53 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 10 | AJ | 87/87 (100%) | 81 (93%) | 6 (7%) | 19 | 15 |
| 10 | BJ | 86/87 (99%) | 68 (79%) | 18 (21%) | 1 | 0 |
| 11 | AK | 90/90 (100%) | 89 (99%) | 1 (1%) | 80 | 85 |
| 11 | BK | 90/90 (100%) | 78 (87%) | 12 (13%) | 5 | 2 |
| 12 | AL | 102/102 (100%) | 101 (99%) | 1 (1%) | 82 | 87 |
| 12 | BL | 102/102 (100%) | 91 (89%) | 11 (11%) | 8 | 4 |
| 13 | AM | 92/92 (100%) | 90 (98%) | 2 (2%) | 60 | 64 |
| 13 | BM | 92/92 (100%) | 79 (86%) | 13 (14%) | 4 | 2 |
| 14 | AN | 83/83 (100%) | 82 (99%) | 1 (1%) | 78 | 84 |
| 14 | BN | 83/83 (100%) | 80 (96%) | 3 (4%) | 42 | 43 |
| 15 | AO | 76/76 (100%) | 74 (97%) | 2 (3%) | 54 | 58 |
| 15 | BO | 76/76 (100%) | 62 (82%) | 14 (18%) | 2 | 1 |
| 16 | AP | 65/65 (100%) | 63 (97%) | 2 (3%) | 47 | 50 |
| 16 | BP | 65/65 (100%) | 58 (89%) | 7 (11%) | 8 | 4 |
| 17 | AQ | 74/74 (100%) | 72 (97%) | 2 (3%) | 52 | 56 |
| 17 | BQ | 74/74 (100%) | 58 (78%) | 16 (22%) | 1 | 0 |
| 18 | AR | 48/48 (100%) | 48 (100%) | 0 | 100 | 100 |
| 18 | BR | 48/48 (100%) | 44 (92%) | 4 (8%) | 14 | 9 |
| 19 | AS | 70/70 (100%) | 69 (99%) | 1 (1%) | 74 | 80 |
| 19 | BS | 70/70 (100%) | 61 (87%) | 9 (13%) | 5 | 2 |
| 20 | AT | 65/65 (100%) | 63 (97%) | 2 (3%) | 47 | 50 |
| 20 | BT | 65/65 (100%) | 53 (82%) | 12 (18%) | 2 | 1 |
| 21 | AU | 48/48 (100%) | 45 (94%) | 3 (6%) | 22 | 18 |
| 21 | BU | 48/48 (100%) | 45 (94%) | 3 (6%) | 22 | 18 |
| 24 | CC | 216/216 (100%) | 194 (90%) | 22 (10%) | 9 | 5 |
| 24 | DC | 216/216 (100%) | 214 (99%) | 2 (1%) | 84 | 89 |
| 25 | CD | 164/164 (100%) | 151 (92%) | 13 (8%) | 15 | 11 |
| 26 | CE | 165/165 (100%) | 144 (87%) | 21 (13%) | 5 | 3 |
| 26 | DE | 165/165 (100%) | 163 (99%) | 2 (1%) | 78 | 84 |
| 27 | CF | 148/148 (100%) | 127 (86%) | 21 (14%) | 4 | 2 |
| 27 | DF | 148/148 (100%) | 142 (96%) | 6 (4%) | 37 | 36 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 28 | CG | 137/137 (100%) | 115 (84%) | 22 (16%) | 3 | 1 |
| 28 | DG | 137/137 (100%) | 129 (94%) | 8 (6%) | 25 | 21 |
| 29 | CH | 114/114 (100%) | 96 (84%) | 18 (16%) | 3 | 1 |
| 29 | DH | 114/114 (100%) | 103 (90%) | 11 (10%) | 10 | 6 |
| 30 | CJ | 104/104 (100%) | 101 (97%) | 3 (3%) | 50 | 53 |
| 30 | DJ | 104/104 (100%) | 103 (99%) | 1 (1%) | 82 | 87 |
| 31 | CK | 116/116 (100%) | 105 (90%) | 11 (10%) | 11 | 7 |
| 31 | DK | 116/116 (100%) | 114 (98%) | 2 (2%) | 68 | 74 |
| 32 | CL | 103/104 (99%) | 96 (93%) | 7 (7%) | 20 | 16 |
| 32 | DL | 104/104 (100%) | 102 (98%) | 2 (2%) | 65 | 70 |
| 33 | CM | 103/103 (100%) | 97 (94%) | 6 (6%) | 25 | 21 |
| 33 | DM | 103/103 (100%) | 102 (99%) | 1 (1%) | 82 | 87 |
| 34 | CN | 108/108 (100%) | 97 (90%) | 11 (10%) | 9 | 5 |
| 34 | DN | 109/108 (101%) | 106 (97%) | 3 (3%) | 51 | 55 |
| 35 | CO | 100/102 (98%) | 87 (87%) | 13 (13%) | 5 | 2 |
| 35 | DO | 102/102 (100%) | 100 (98%) | 2 (2%) | 63 | 68 |
| 36 | CP | 86/87 (99%) | 76 (88%) | 10 (12%) | 7 | 3 |
| 36 | DP | 87/87 (100%) | 85 (98%) | 2 (2%) | 58 | 62 |
| 37 | CQ | 99/99 (100%) | 89 (90%) | 10 (10%) | 9 | 5 |
| 37 | DQ | 99/99 (100%) | 95 (96%) | 4 (4%) | 38 | 38 |
| 38 | CR | 89/89 (100%) | 81 (91%) | 8 (9%) | 12 | 8 |
| 38 | DR | 89/89 (100%) | 87 (98%) | 2 (2%) | 60 | 64 |
| 39 | CS | 84/84 (100%) | 74 (88%) | 10 (12%) | 6 | 3 |
| 39 | DS | 84/84 (100%) | 81 (96%) | 3 (4%) | 42 | 43 |
| 40 | CT | 93/93 (100%) | 79 (85%) | 14 (15%) | 3 | 1 |
| 40 | DT | 93/93 (100%) | 91 (98%) | 2 (2%) | 60 | 64 |
| 41 | CU | 80/80 (100%) | 66 (82%) | 14 (18%) | 2 | 1 |
| 41 | DU | 80/80 (100%) | 77 (96%) | 3 (4%) | 40 | 40 |
| 42 | CV | 83/83 (100%) | 71 (86%) | 12 (14%) | 4 | 2 |
| 42 | DV | 83/83 (100%) | 82 (99%) | 1 (1%) | 78 | 84 |
| 43 | CW | 78/78 (100%) | 65 (83%) | 13 (17%) | 3 | 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|-----|
| 43 | DW | 78/78 (100%) | 75 (96%) | 3 (4%) | 40 | 40 |
| 44 | CX | 56/58 (97%) | 53 (95%) | 3 (5%) | 27 | 24 |
| 44 | DX | 58/58 (100%) | 57 (98%) | 1 (2%) | 68 | 74 |
| 45 | CY | 67/67 (100%) | 60 (90%) | 7 (10%) | 9 | 5 |
| 45 | DY | 67/67 (100%) | 66 (98%) | 1 (2%) | 72 | 78 |
| 46 | CZ | 54/54 (100%) | 47 (87%) | 7 (13%) | 5 | 2 |
| 46 | DZ | 54/54 (100%) | 54 (100%) | 0 | 100 | 100 |
| 47 | C0 | 48/48 (100%) | 42 (88%) | 6 (12%) | 6 | 3 |
| 47 | D0 | 49/48 (102%) | 48 (98%) | 1 (2%) | 63 | 68 |
| 48 | C1 | 47/47 (100%) | 43 (92%) | 4 (8%) | 13 | 9 |
| 48 | D1 | 47/47 (100%) | 47 (100%) | 0 | 100 | 100 |
| 49 | C2 | 45/46 (98%) | 44 (98%) | 1 (2%) | 60 | 64 |
| 49 | D2 | 45/46 (98%) | 45 (100%) | 0 | 100 | 100 |
| 50 | C3 | 38/38 (100%) | 34 (90%) | 4 (10%) | 8 | 5 |
| 50 | D3 | 38/38 (100%) | 37 (97%) | 1 (3%) | 54 | 58 |
| 51 | C4 | 51/51 (100%) | 47 (92%) | 4 (8%) | 16 | 11 |
| 51 | D4 | 51/51 (100%) | 50 (98%) | 1 (2%) | 63 | 68 |
| 52 | C5 | 34/34 (100%) | 32 (94%) | 2 (6%) | 24 | 20 |
| 52 | D5 | 34/34 (100%) | 34 (100%) | 0 | 100 | 100 |
| 54 | DD | 163/163 (100%) | 161 (99%) | 2 (1%) | 78 | 84 |
| 55 | DI | 103/103 (100%) | 100 (97%) | 3 (3%) | 50 | 53 |
| All | All | 9461/9478 (100%) | 8793 (93%) | 668 (7%) | 18 | 14 |

All (668) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | AB | 5 | SER |
| 2 | AB | 23 | TRP |
| 2 | AB | 73 | LYS |
| 2 | AB | 93 | ASN |
| 2 | AB | 129 | LEU |
| 2 | AB | 213 | TYR |
| 3 | AC | 20 | SER |
| 3 | AC | 58 | GLU |
| 3 | AC | 83 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | AC | 85 | GLU |
| 3 | AC | 125 | GLU |
| 3 | AC | 201 | TRP |
| 4 | AD | 26 | ARG |
| 4 | AD | 131 | ASN |
| 4 | AD | 194 | ASP |
| 4 | AD | 196 | ASN |
| 4 | AD | 197 | GLU |
| 5 | AE | 22 | SER |
| 5 | AE | 48 | PHE |
| 5 | AE | 80 | THR |
| 5 | AE | 130 | SER |
| 5 | AE | 152 | MET |
| 5 | AE | 163 | GLU |
| 6 | AF | 93 | LYS |
| 7 | AG | 7 | ILE |
| 7 | AG | 54 | SER |
| 7 | AG | 83 | SER |
| 8 | AH | 3 | MET |
| 8 | AH | 60 | GLU |
| 8 | AH | 75 | ILE |
| 8 | AH | 107 | SER |
| 9 | AI | 47 | VAL |
| 9 | AI | 66 | THR |
| 9 | AI | 94 | LEU |
| 10 | AJ | 7 | ARG |
| 10 | AJ | 16 | ARG |
| 10 | AJ | 19 | ASP |
| 10 | AJ | 27 | GLU |
| 10 | AJ | 35 | GLN |
| 10 | AJ | 80 | THR |
| 11 | AK | 33 | THR |
| 12 | AL | 15 | LYS |
| 13 | AM | 71 | ARG |
| 13 | AM | 107 | ARG |
| 14 | AN | 59 | ARG |
| 15 | AO | 3 | LEU |
| 15 | AO | 89 | ARG |
| 16 | AP | 1 | MET |
| 16 | AP | 44 | SER |
| 17 | AQ | 14 | SER |
| 17 | AQ | 27 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19 | AS | 18 | LYS |
| 20 | AT | 40 | GLU |
| 20 | AT | 54 | MET |
| 21 | AU | 4 | ILE |
| 21 | AU | 41 | PRO |
| 21 | AU | 56 | HIS |
| 2 | BB | 5 | SER |
| 2 | BB | 23 | TRP |
| 2 | BB | 73 | LYS |
| 2 | BB | 93 | ASN |
| 2 | BB | 129 | LEU |
| 2 | BB | 146 | ASN |
| 2 | BB | 213 | TYR |
| 3 | BC | 3 | GLN |
| 3 | BC | 20 | SER |
| 3 | BC | 27 | LYS |
| 3 | BC | 38 | LYS |
| 3 | BC | 43 | LEU |
| 3 | BC | 55 | ILE |
| 3 | BC | 58 | GLU |
| 3 | BC | 59 | ARG |
| 3 | BC | 75 | ILE |
| 3 | BC | 80 | LYS |
| 3 | BC | 82 | GLU |
| 3 | BC | 86 | LYS |
| 3 | BC | 89 | LYS |
| 3 | BC | 103 | ILE |
| 3 | BC | 107 | ARG |
| 3 | BC | 125 | GLU |
| 3 | BC | 127 | ARG |
| 3 | BC | 140 | ASN |
| 3 | BC | 152 | GLU |
| 3 | BC | 157 | LEU |
| 3 | BC | 165 | THR |
| 3 | BC | 169 | ARG |
| 3 | BC | 175 | LEU |
| 3 | BC | 179 | ARG |
| 3 | BC | 192 | THR |
| 3 | BC | 200 | VAL |
| 3 | BC | 201 | TRP |
| 3 | BC | 206 | GLU |
| 4 | BD | 5 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | BD | 58 | LYS |
| 4 | BD | 142 | VAL |
| 4 | BD | 196 | ASN |
| 4 | BD | 206 | LYS |
| 5 | BE | 11 | LEU |
| 5 | BE | 12 | GLN |
| 5 | BE | 15 | LEU |
| 5 | BE | 22 | SER |
| 5 | BE | 26 | LYS |
| 5 | BE | 38 | VAL |
| 5 | BE | 52 | LYS |
| 5 | BE | 69 | ARG |
| 5 | BE | 78 | ASN |
| 5 | BE | 80 | THR |
| 5 | BE | 81 | LEU |
| 5 | BE | 93 | ARG |
| 5 | BE | 96 | MET |
| 5 | BE | 101 | GLU |
| 5 | BE | 105 | ILE |
| 5 | BE | 115 | LEU |
| 5 | BE | 120 | VAL |
| 5 | BE | 122 | ASN |
| 5 | BE | 130 | SER |
| 5 | BE | 149 | SER |
| 5 | BE | 151 | GLU |
| 6 | BF | 14 | GLN |
| 6 | BF | 16 | GLU |
| 6 | BF | 29 | ILE |
| 6 | BF | 35 | LYS |
| 6 | BF | 51 | ILE |
| 6 | BF | 53 | LYS |
| 6 | BF | 54 | LEU |
| 6 | BF | 56 | LYS |
| 6 | BF | 68 | GLN |
| 6 | BF | 69 | GLU |
| 6 | BF | 77 | THR |
| 6 | BF | 79 | ARG |
| 6 | BF | 86 | ARG |
| 6 | BF | 93 | LYS |
| 7 | BG | 3 | ARG |
| 7 | BG | 4 | ARG |
| 7 | BG | 5 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | BG | 11 | LYS |
| 7 | BG | 12 | ILE |
| 7 | BG | 15 | ASP |
| 7 | BG | 22 | LEU |
| 7 | BG | 29 | ILE |
| 7 | BG | 47 | LEU |
| 7 | BG | 59 | LEU |
| 7 | BG | 60 | GLU |
| 7 | BG | 63 | GLU |
| 7 | BG | 66 | LEU |
| 7 | BG | 73 | VAL |
| 7 | BG | 77 | SER |
| 7 | BG | 78 | ARG |
| 7 | BG | 79 | ARG |
| 7 | BG | 89 | VAL |
| 7 | BG | 92 | ARG |
| 7 | BG | 97 | ASN |
| 7 | BG | 113 | ASP |
| 7 | BG | 123 | GLU |
| 7 | BG | 129 | GLU |
| 7 | BG | 136 | LYS |
| 7 | BG | 140 | ASP |
| 7 | BG | 143 | ARG |
| 7 | BG | 144 | MET |
| 8 | BH | 3 | MET |
| 8 | BH | 18 | GLN |
| 8 | BH | 25 | VAL |
| 8 | BH | 26 | THR |
| 8 | BH | 51 | VAL |
| 8 | BH | 52 | GLU |
| 8 | BH | 59 | LEU |
| 8 | BH | 75 | ILE |
| 8 | BH | 77 | ARG |
| 8 | BH | 83 | LEU |
| 8 | BH | 87 | LYS |
| 8 | BH | 90 | ASP |
| 8 | BH | 107 | SER |
| 8 | BH | 111 | MET |
| 8 | BH | 114 | ARG |
| 8 | BH | 121 | LEU |
| 8 | BH | 125 | ILE |
| 9 | BI | 47 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | BI | 66 | THR |
| 9 | BI | 94 | LEU |
| 10 | BJ | 5 | ARG |
| 10 | BJ | 9 | ARG |
| 10 | BJ | 16 | ARG |
| 10 | BJ | 22 | THR |
| 10 | BJ | 24 | GLU |
| 10 | BJ | 25 | ILE |
| 10 | BJ | 37 | ARG |
| 10 | BJ | 51 | VAL |
| 10 | BJ | 62 | ARG |
| 10 | BJ | 63 | ASP |
| 10 | BJ | 69 | THR |
| 10 | BJ | 73 | LEU |
| 10 | BJ | 77 | VAL |
| 10 | BJ | 82 | LYS |
| 10 | BJ | 88 | MET |
| 10 | BJ | 90 | LEU |
| 10 | BJ | 99 | GLN |
| 10 | BJ | 100 | ILE |
| 11 | BK | 31 | ILE |
| 11 | BK | 38 | GLN |
| 11 | BK | 55 | SER |
| 11 | BK | 57 | LYS |
| 11 | BK | 82 | LEU |
| 11 | BK | 83 | GLU |
| 11 | BK | 100 | LEU |
| 11 | BK | 105 | PHE |
| 11 | BK | 107 | ILE |
| 11 | BK | 109 | ASN |
| 11 | BK | 114 | THR |
| 11 | BK | 122 | ARG |
| 12 | BL | 9 | ARG |
| 12 | BL | 10 | LYS |
| 12 | BL | 12 | ARG |
| 12 | BL | 14 | ARG |
| 12 | BL | 44 | LYS |
| 12 | BL | 49 | LEU |
| 12 | BL | 54 | ARG |
| 12 | BL | 58 | THR |
| 12 | BL | 88 | LYS |
| 12 | BL | 94 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | BL | 121 | ARG |
| 13 | BM | 4 | ILE |
| 13 | BM | 16 | VAL |
| 13 | BM | 23 | TYR |
| 13 | BM | 27 | LYS |
| 13 | BM | 29 | ARG |
| 13 | BM | 31 | LYS |
| 13 | BM | 48 | LEU |
| 13 | BM | 59 | GLU |
| 13 | BM | 90 | ARG |
| 13 | BM | 91 | HIS |
| 13 | BM | 107 | ARG |
| 13 | BM | 110 | LYS |
| 13 | BM | 114 | LYS |
| 14 | BN | 26 | GLU |
| 14 | BN | 32 | SER |
| 14 | BN | 59 | ARG |
| 15 | BO | 6 | GLU |
| 15 | BO | 8 | THR |
| 15 | BO | 17 | ARG |
| 15 | BO | 18 | ASP |
| 15 | BO | 35 | GLN |
| 15 | BO | 39 | LEU |
| 15 | BO | 64 | ARG |
| 15 | BO | 70 | LEU |
| 15 | BO | 73 | LYS |
| 15 | BO | 83 | GLU |
| 15 | BO | 85 | LEU |
| 15 | BO | 87 | LEU |
| 15 | BO | 88 | ARG |
| 15 | BO | 89 | ARG |
| 16 | BP | 1 | MET |
| 16 | BP | 18 | GLN |
| 16 | BP | 20 | VAL |
| 16 | BP | 46 | LYS |
| 16 | BP | 51 | ARG |
| 16 | BP | 63 | GLN |
| 16 | BP | 68 | SER |
| 17 | BQ | 5 | ILE |
| 17 | BQ | 7 | THR |
| 17 | BQ | 14 | SER |
| 17 | BQ | 16 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 17 | BQ | 17 | MET |
| 17 | BQ | 22 | VAL |
| 17 | BQ | 26 | GLU |
| 17 | BQ | 29 | VAL |
| 17 | BQ | 40 | ARG |
| 17 | BQ | 55 | ILE |
| 17 | BQ | 61 | ILE |
| 17 | BQ | 65 | ARG |
| 17 | BQ | 75 | LEU |
| 17 | BQ | 76 | VAL |
| 17 | BQ | 79 | VAL |
| 17 | BQ | 81 | LYS |
| 18 | BR | 21 | ILE |
| 18 | BR | 47 | THR |
| 18 | BR | 55 | LEU |
| 18 | BR | 73 | ARG |
| 19 | BS | 6 | LYS |
| 19 | BS | 7 | LYS |
| 19 | BS | 11 | ILE |
| 19 | BS | 13 | LEU |
| 19 | BS | 33 | THR |
| 19 | BS | 37 | ARG |
| 19 | BS | 49 | ILE |
| 19 | BS | 58 | VAL |
| 19 | BS | 80 | TYR |
| 20 | BT | 10 | ARG |
| 20 | BT | 12 | ILE |
| 20 | BT | 24 | ARG |
| 20 | BT | 27 | MET |
| 20 | BT | 30 | THR |
| 20 | BT | 36 | TYR |
| 20 | BT | 54 | MET |
| 20 | BT | 64 | LYS |
| 20 | BT | 66 | LEU |
| 20 | BT | 69 | LYS |
| 20 | BT | 84 | ASN |
| 20 | BT | 86 | LEU |
| 21 | BU | 12 | PHE |
| 21 | BU | 34 | ARG |
| 21 | BU | 56 | HIS |
| 24 | CC | 14 | ARG |
| 24 | CC | 18 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24 | CC | 36 | LYS |
| 24 | CC | 52 | ARG |
| 24 | CC | 88 | SER |
| 24 | CC | 97 | LYS |
| 24 | CC | 105 | LEU |
| 24 | CC | 130 | LEU |
| 24 | CC | 139 | SER |
| 24 | CC | 141 | VAL |
| 24 | CC | 156 | ARG |
| 24 | CC | 157 | SER |
| 24 | CC | 168 | ASP |
| 24 | CC | 174 | LEU |
| 24 | CC | 187 | ASP |
| 24 | CC | 195 | VAL |
| 24 | CC | 203 | ARG |
| 24 | CC | 204 | VAL |
| 24 | CC | 213 | TRP |
| 24 | CC | 265 | LYS |
| 24 | CC | 267 | ILE |
| 24 | CC | 269 | ARG |
| 25 | CD | 4 | LEU |
| 25 | CD | 12 | THR |
| 25 | CD | 32 | ASN |
| 25 | CD | 33 | ARG |
| 25 | CD | 39 | ASP |
| 25 | CD | 46 | ARG |
| 25 | CD | 73 | VAL |
| 25 | CD | 91 | THR |
| 25 | CD | 95 | SER |
| 25 | CD | 150 | GLN |
| 25 | CD | 157 | LYS |
| 25 | CD | 170 | VAL |
| 25 | CD | 177 | VAL |
| 26 | CE | 12 | LEU |
| 26 | CE | 25 | GLU |
| 26 | CE | 44 | ARG |
| 26 | CE | 57 | LYS |
| 26 | CE | 65 | THR |
| 26 | CE | 67 | ARG |
| 26 | CE | 69 | ARG |
| 26 | CE | 72 | SER |
| 26 | CE | 78 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26 | CE | 88 | ARG |
| 26 | CE | 93 | SER |
| 26 | CE | 116 | ASP |
| 26 | CE | 126 | VAL |
| 26 | CE | 133 | LEU |
| 26 | CE | 139 | LYS |
| 26 | CE | 146 | VAL |
| 26 | CE | 149 | ILE |
| 26 | CE | 150 | THR |
| 26 | CE | 164 | LEU |
| 26 | CE | 187 | VAL |
| 26 | CE | 200 | LEU |
| 27 | CF | 3 | LYS |
| 27 | CF | 5 | HIS |
| 27 | CF | 7 | TYR |
| 27 | CF | 18 | THR |
| 27 | CF | 19 | GLU |
| 27 | CF | 21 | ASN |
| 27 | CF | 26 | MET |
| 27 | CF | 31 | VAL |
| 27 | CF | 35 | THR |
| 27 | CF | 36 | LEU |
| 27 | CF | 46 | ASP |
| 27 | CF | 64 | LYS |
| 27 | CF | 80 | ARG |
| 27 | CF | 95 | ARG |
| 27 | CF | 104 | ILE |
| 27 | CF | 117 | LEU |
| 27 | CF | 141 | ILE |
| 27 | CF | 148 | ARG |
| 27 | CF | 149 | VAL |
| 27 | CF | 154 | ILE |
| 27 | CF | 174 | ASP |
| 28 | CG | 11 | VAL |
| 28 | CG | 25 | THR |
| 28 | CG | 27 | LYS |
| 28 | CG | 29 | LYS |
| 28 | CG | 30 | ASN |
| 28 | CG | 34 | THR |
| 28 | CG | 37 | LEU |
| 28 | CG | 44 | LYS |
| 28 | CG | 45 | HIS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 28 | CG | 49 | THR |
| 28 | CG | 73 | ASN |
| 28 | CG | 74 | SER |
| 28 | CG | 80 | THR |
| 28 | CG | 92 | VAL |
| 28 | CG | 98 | VAL |
| 28 | CG | 117 | LEU |
| 28 | CG | 124 | GLU |
| 28 | CG | 127 | THR |
| 28 | CG | 137 | ASP |
| 28 | CG | 155 | GLU |
| 28 | CG | 166 | ASP |
| 28 | CG | 168 | VAL |
| 29 | CH | 3 | VAL |
| 29 | CH | 6 | LEU |
| 29 | CH | 11 | ASN |
| 29 | CH | 12 | LEU |
| 29 | CH | 14 | SER |
| 29 | CH | 17 | ASP |
| 29 | CH | 41 | LYS |
| 29 | CH | 42 | LYS |
| 29 | CH | 51 | ARG |
| 29 | CH | 72 | ILE |
| 29 | CH | 75 | LEU |
| 29 | CH | 78 | VAL |
| 29 | CH | 87 | GLU |
| 29 | CH | 97 | ARG |
| 29 | CH | 101 | ASP |
| 29 | CH | 124 | THR |
| 29 | CH | 142 | VAL |
| 29 | CH | 144 | VAL |
| 30 | CJ | 59 | ILE |
| 30 | CJ | 82 | LYS |
| 30 | CJ | 103 | ARG |
| 31 | CK | 3 | THR |
| 31 | CK | 28 | LEU |
| 31 | CK | 30 | THR |
| 31 | CK | 39 | LYS |
| 31 | CK | 57 | LEU |
| 31 | CK | 95 | ARG |
| 31 | CK | 123 | LYS |
| 31 | CK | 124 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 31 | CK | 129 | GLU |
| 31 | CK | 131 | ASN |
| 31 | CK | 142 | ILE |
| 32 | CL | 49 | ARG |
| 32 | CL | 76 | VAL |
| 32 | CL | 90 | ASN |
| 32 | CL | 92 | GLU |
| 32 | CL | 105 | ARG |
| 32 | CL | 107 | LEU |
| 32 | CL | 114 | LYS |
| 33 | CM | 82 | LEU |
| 33 | CM | 92 | LEU |
| 33 | CM | 94 | THR |
| 33 | CM | 100 | ILE |
| 33 | CM | 115 | GLU |
| 33 | CM | 118 | THR |
| 34 | CN | 18 | ARG |
| 34 | CN | 20 | LEU |
| 34 | CN | 24 | THR |
| 34 | CN | 27 | SER |
| 34 | CN | 40 | ARG |
| 34 | CN | 53 | MET |
| 34 | CN | 58 | LYS |
| 34 | CN | 59 | ARG |
| 34 | CN | 78 | LEU |
| 34 | CN | 100 | LYS |
| 34 | CN | 111 | GLU |
| 35 | CO | 1 | MET |
| 35 | CO | 2 | ARG |
| 35 | CO | 20 | MET |
| 35 | CO | 51 | LEU |
| 35 | CO | 63 | ARG |
| 35 | CO | 70 | THR |
| 35 | CO | 71 | ARG |
| 35 | CO | 76 | VAL |
| 35 | CO | 90 | ARG |
| 35 | CO | 95 | THR |
| 35 | CO | 116 | VAL |
| 35 | CO | 118 | ARG |
| 35 | CO | 119 | SER |
| 36 | CP | 9 | ARG |
| 36 | CP | 16 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36 | CP | 18 | LEU |
| 36 | CP | 25 | ARG |
| 36 | CP | 31 | THR |
| 36 | CP | 38 | GLN |
| 36 | CP | 47 | VAL |
| 36 | CP | 78 | VAL |
| 36 | CP | 94 | ARG |
| 36 | CP | 103 | VAL |
| 37 | CQ | 6 | LYS |
| 37 | CQ | 8 | LEU |
| 37 | CQ | 19 | SER |
| 37 | CQ | 37 | LYS |
| 37 | CQ | 39 | ARG |
| 37 | CQ | 40 | LEU |
| 37 | CQ | 72 | ARG |
| 37 | CQ | 73 | VAL |
| 37 | CQ | 80 | VAL |
| 37 | CQ | 110 | ILE |
| 38 | CR | 5 | LYS |
| 38 | CR | 9 | ILE |
| 38 | CR | 11 | ARG |
| 38 | CR | 13 | ARG |
| 38 | CR | 16 | LYS |
| 38 | CR | 41 | LYS |
| 38 | CR | 51 | ARG |
| 38 | CR | 58 | ARG |
| 39 | CS | 10 | LYS |
| 39 | CS | 38 | VAL |
| 39 | CS | 45 | GLU |
| 39 | CS | 46 | GLU |
| 39 | CS | 47 | VAL |
| 39 | CS | 48 | LYS |
| 39 | CS | 58 | VAL |
| 39 | CS | 60 | LYS |
| 39 | CS | 62 | GLU |
| 39 | CS | 102 | SER |
| 40 | CT | 7 | HIS |
| 40 | CT | 13 | SER |
| 40 | CT | 19 | LEU |
| 40 | CT | 30 | SER |
| 40 | CT | 65 | ASP |
| 40 | CT | 66 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40 | CT | 69 | LEU |
| 40 | CT | 76 | VAL |
| 40 | CT | 86 | MET |
| 40 | CT | 96 | ILE |
| 40 | CT | 97 | LEU |
| 40 | CT | 107 | VAL |
| 40 | CT | 109 | ASP |
| 40 | CT | 110 | ARG |
| 41 | CU | 2 | ILE |
| 41 | CU | 3 | ARG |
| 41 | CU | 5 | GLU |
| 41 | CU | 18 | GLU |
| 41 | CU | 22 | THR |
| 41 | CU | 30 | ILE |
| 41 | CU | 49 | LYS |
| 41 | CU | 50 | LEU |
| 41 | CU | 56 | GLU |
| 41 | CU | 68 | LYS |
| 41 | CU | 69 | ARG |
| 41 | CU | 70 | HIS |
| 41 | CU | 73 | ARG |
| 41 | CU | 77 | ARG |
| 42 | CV | 7 | ARG |
| 42 | CV | 19 | LYS |
| 42 | CV | 29 | LEU |
| 42 | CV | 35 | ILE |
| 42 | CV | 37 | GLU |
| 42 | CV | 41 | LEU |
| 42 | CV | 53 | ASN |
| 42 | CV | 61 | LYS |
| 42 | CV | 68 | SER |
| 42 | CV | 72 | ILE |
| 42 | CV | 74 | ASN |
| 42 | CV | 101 | GLU |
| 43 | CW | 1 | MET |
| 43 | CW | 7 | GLU |
| 43 | CW | 10 | LYS |
| 43 | CW | 20 | LEU |
| 43 | CW | 34 | LYS |
| 43 | CW | 40 | ILE |
| 43 | CW | 41 | GLU |
| 43 | CW | 53 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43 | CW | 61 | LEU |
| 43 | CW | 62 | THR |
| 43 | CW | 65 | VAL |
| 43 | CW | 70 | ILE |
| 43 | CW | 76 | ASP |
| 44 | CX | 30 | SER |
| 44 | CX | 38 | VAL |
| 44 | CX | 77 | ARG |
| 45 | CY | 17 | ASN |
| 45 | CY | 20 | HIS |
| 45 | CY | 22 | LEU |
| 45 | CY | 35 | SER |
| 45 | CY | 48 | THR |
| 45 | CY | 71 | LEU |
| 45 | CY | 72 | ARG |
| 46 | CZ | 7 | ARG |
| 46 | CZ | 18 | LEU |
| 46 | CZ | 19 | LEU |
| 46 | CZ | 21 | LEU |
| 46 | CZ | 38 | GLN |
| 46 | CZ | 57 | LEU |
| 46 | CZ | 58 | ASN |
| 47 | C0 | 3 | LYS |
| 47 | C0 | 4 | THR |
| 47 | C0 | 5 | ILE |
| 47 | C0 | 10 | THR |
| 47 | C0 | 19 | LYS |
| 47 | C0 | 57 | VAL |
| 48 | C1 | 10 | ARG |
| 48 | C1 | 26 | THR |
| 48 | C1 | 28 | LEU |
| 48 | C1 | 40 | ARG |
| 49 | C2 | 47 | VAL |
| 50 | C3 | 1 | MET |
| 50 | C3 | 3 | ARG |
| 50 | C3 | 4 | THR |
| 50 | C3 | 42 | LEU |
| 51 | C4 | 19 | LYS |
| 51 | C4 | 30 | ARG |
| 51 | C4 | 31 | HIS |
| 51 | C4 | 47 | LYS |
| 52 | C5 | 3 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52 | C5 | 26 | ILE |
| 24 | DC | 130 | LEU |
| 24 | DC | 252 | THR |
| 54 | DD | 32 | ASN |
| 54 | DD | 95 | SER |
| 26 | DE | 7 | ASP |
| 26 | DE | 116 | ASP |
| 27 | DF | 95 | ARG |
| 27 | DF | 105 | THR |
| 27 | DF | 113 | ASP |
| 27 | DF | 144 | ASP |
| 27 | DF | 154 | ILE |
| 27 | DF | 174 | ASP |
| 28 | DG | 45 | HIS |
| 28 | DG | 77 | ILE |
| 28 | DG | 81 | GLU |
| 28 | DG | 85 | LYS |
| 28 | DG | 104 | ASN |
| 28 | DG | 114 | ASP |
| 28 | DG | 152 | ARG |
| 28 | DG | 177 | LYS |
| 29 | DH | 8 | LYS |
| 29 | DH | 14 | SER |
| 29 | DH | 42 | LYS |
| 29 | DH | 44 | ILE |
| 29 | DH | 46 | PHE |
| 29 | DH | 50 | ARG |
| 29 | DH | 53 | GLU |
| 29 | DH | 60 | GLU |
| 29 | DH | 76 | GLU |
| 29 | DH | 77 | THR |
| 29 | DH | 125 | THR |
| 55 | DI | 16 | SER |
| 55 | DI | 71 | CYS |
| 55 | DI | 105 | LYS |
| 30 | DJ | 59 | ILE |
| 31 | DK | 39 | LYS |
| 31 | DK | 124 | VAL |
| 32 | DL | 49 | ARG |
| 32 | DL | 58 | LEU |
| 33 | DM | 115 | GLU |
| 34 | DN | 27 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34 | DN | 59 | ARG |
| 34 | DN | 135 | VAL |
| 35 | DO | 75 | ILE |
| 35 | DO | 116 | VAL |
| 36 | DP | 31 | THR |
| 36 | DP | 78 | VAL |
| 37 | DQ | 19 | SER |
| 37 | DQ | 68 | GLU |
| 37 | DQ | 85 | SER |
| 37 | DQ | 96 | LYS |
| 38 | DR | 11 | ARG |
| 38 | DR | 51 | ARG |
| 39 | DS | 38 | VAL |
| 39 | DS | 45 | GLU |
| 39 | DS | 102 | SER |
| 40 | DT | 86 | MET |
| 40 | DT | 109 | ASP |
| 41 | DU | 5 | GLU |
| 41 | DU | 92 | ASN |
| 41 | DU | 93 | LEU |
| 42 | DV | 55 | PRO |
| 43 | DW | 7 | GLU |
| 43 | DW | 66 | ASP |
| 43 | DW | 70 | ILE |
| 44 | DX | 11 | ARG |
| 45 | DY | 2 | SER |
| 47 | D0 | 10 | THR |
| 50 | D3 | 1 | MET |
| 51 | D4 | 31 | HIS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | AG | 52 | GLN |
| 26 | CE | 115 | GLN |
| 30 | CJ | 31 | GLN |

5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1 | AA | 1530/1534 (99%) | 258 (16%) | 9 (0%) |
| 1 | BA | 1529/1534 (99%) | 267 (17%) | 10 (0%) |
| 22 | CA | 2892/2904 (99%) | 414 (14%) | 32 (1%) |
| 23 | CB | 117/120 (97%) | 11 (9%) | 0 |
| 23 | DB | 119/120 (99%) | 8 (6%) | 0 |
| 53 | DA | 2883/2903 (99%) | 377 (13%) | 26 (0%) |
| All | All | 9070/9115 (99%) | 1335 (14%) | 77 (0%) |

All (1335) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 5 | U |
| 1 | AA | 6 | G |
| 1 | AA | 9 | G |
| 1 | AA | 22 | G |
| 1 | AA | 28 | A |
| 1 | AA | 32 | A |
| 1 | AA | 39 | G |
| 1 | AA | 47 | C |
| 1 | AA | 48 | C |
| 1 | AA | 50 | A |
| 1 | AA | 51 | A |
| 1 | AA | 69 | G |
| 1 | AA | 70 | U |
| 1 | AA | 71 | A |
| 1 | AA | 72 | A |
| 1 | AA | 73 | C |
| 1 | AA | 74 | A |
| 1 | AA | 75 | G |
| 1 | AA | 76 | G |
| 1 | AA | 77 | A |
| 1 | AA | 78 | A |
| 1 | AA | 79 | G |
| 1 | AA | 80 | A |
| 1 | AA | 81 | A |
| 1 | AA | 82 | G |
| 1 | AA | 83 | C |
| 1 | AA | 84 | U |
| 1 | AA | 85 | U |
| 1 | AA | 86 | G |
| 1 | AA | 89 | U |
| 1 | AA | 90 | C |
| 1 | AA | 91 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 94 | G |
| 1 | AA | 95 | C |
| 1 | AA | 97 | G |
| 1 | AA | 108 | G |
| 1 | AA | 119 | A |
| 1 | AA | 121 | U |
| 1 | AA | 122 | G |
| 1 | AA | 128 | G |
| 1 | AA | 130 | A |
| 1 | AA | 131 | A |
| 1 | AA | 137 | U |
| 1 | AA | 142 | G |
| 1 | AA | 144 | G |
| 1 | AA | 158 | G |
| 1 | AA | 159 | G |
| 1 | AA | 163 | C |
| 1 | AA | 168 | G |
| 1 | AA | 173 | U |
| 1 | AA | 183 | C |
| 1 | AA | 201 | G |
| 1 | AA | 205 | A |
| 1 | AA | 208 | U |
| 1 | AA | 209 | U |
| 1 | AA | 210 | C |
| 1 | AA | 212 | G |
| 1 | AA | 240 | G |
| 1 | AA | 245 | U |
| 1 | AA | 247 | G |
| 1 | AA | 251 | G |
| 1 | AA | 262 | A |
| 1 | AA | 266 | G |
| 1 | AA | 267 | C |
| 1 | AA | 289 | G |
| 1 | AA | 321 | A |
| 1 | AA | 328 | C |
| 1 | AA | 329 | A |
| 1 | AA | 330 | C |
| 1 | AA | 332 | G |
| 1 | AA | 346 | G |
| 1 | AA | 352 | C |
| 1 | AA | 354 | G |
| 1 | AA | 367 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 372 | C |
| 1 | AA | 373 | A |
| 1 | AA | 382 | A |
| 1 | AA | 384 | G |
| 1 | AA | 406 | G |
| 1 | AA | 411 | A |
| 1 | AA | 412 | A |
| 1 | AA | 413 | G |
| 1 | AA | 421 | U |
| 1 | AA | 422 | C |
| 1 | AA | 429 | U |
| 1 | AA | 430 | A |
| 1 | AA | 435 | A |
| 1 | AA | 439 | U |
| 1 | AA | 444 | G |
| 1 | AA | 457 | G |
| 1 | AA | 458 | U |
| 1 | AA | 463 | U |
| 1 | AA | 466 | A |
| 1 | AA | 467 | U |
| 1 | AA | 468 | A |
| 1 | AA | 481 | G |
| 1 | AA | 486 | U |
| 1 | AA | 495 | A |
| 1 | AA | 496 | A |
| 1 | AA | 509 | A |
| 1 | AA | 511 | C |
| 1 | AA | 512 | U |
| 1 | AA | 527 | G7M |
| 1 | AA | 530 | G |
| 1 | AA | 532 | A |
| 1 | AA | 533 | A |
| 1 | AA | 547 | A |
| 1 | AA | 559 | A |
| 1 | AA | 562 | U |
| 1 | AA | 564 | C |
| 1 | AA | 572 | A |
| 1 | AA | 573 | A |
| 1 | AA | 576 | C |
| 1 | AA | 577 | G |
| 1 | AA | 631 | C |
| 1 | AA | 632 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 649 | A |
| 1 | AA | 650 | G |
| 1 | AA | 653 | U |
| 1 | AA | 665 | A |
| 1 | AA | 682 | G |
| 1 | AA | 721 | G |
| 1 | AA | 723 | U |
| 1 | AA | 724 | G |
| 1 | AA | 733 | G |
| 1 | AA | 753 | A |
| 1 | AA | 755 | G |
| 1 | AA | 777 | A |
| 1 | AA | 793 | U |
| 1 | AA | 794 | A |
| 1 | AA | 815 | A |
| 1 | AA | 817 | C |
| 1 | AA | 827 | U |
| 1 | AA | 828 | U |
| 1 | AA | 832 | G |
| 1 | AA | 841 | C |
| 1 | AA | 842 | U |
| 1 | AA | 843 | U |
| 1 | AA | 845 | A |
| 1 | AA | 846 | G |
| 1 | AA | 887 | G |
| 1 | AA | 913 | A |
| 1 | AA | 914 | A |
| 1 | AA | 926 | G |
| 1 | AA | 927 | G |
| 1 | AA | 932 | C |
| 1 | AA | 934 | C |
| 1 | AA | 960 | U |
| 1 | AA | 969 | A |
| 1 | AA | 975 | A |
| 1 | AA | 976 | G |
| 1 | AA | 977 | A |
| 1 | AA | 992 | U |
| 1 | AA | 993 | G |
| 1 | AA | 1004 | A |
| 1 | AA | 1005 | A |
| 1 | AA | 1009 | U |
| 1 | AA | 1012 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1015 | G |
| 1 | AA | 1017 | U |
| 1 | AA | 1019 | A |
| 1 | AA | 1021 | A |
| 1 | AA | 1022 | A |
| 1 | AA | 1023 | U |
| 1 | AA | 1025 | U |
| 1 | AA | 1026 | G |
| 1 | AA | 1027 | C |
| 1 | AA | 1028 | C |
| 1 | AA | 1029 | U |
| 1 | AA | 1030 | U |
| 1 | AA | 1031 | C |
| 1 | AA | 1032 | G |
| 1 | AA | 1033 | G |
| 1 | AA | 1034 | G |
| 1 | AA | 1036 | A |
| 1 | AA | 1037 | C |
| 1 | AA | 1043 | G |
| 1 | AA | 1053 | G |
| 1 | AA | 1054 | C |
| 1 | AA | 1065 | U |
| 1 | AA | 1070 | U |
| 1 | AA | 1086 | U |
| 1 | AA | 1092 | A |
| 1 | AA | 1094 | G |
| 1 | AA | 1095 | U |
| 1 | AA | 1098 | C |
| 1 | AA | 1101 | A |
| 1 | AA | 1108 | G |
| 1 | AA | 1124 | G |
| 1 | AA | 1133 | G |
| 1 | AA | 1135 | U |
| 1 | AA | 1136 | C |
| 1 | AA | 1137 | C |
| 1 | AA | 1138 | G |
| 1 | AA | 1139 | G |
| 1 | AA | 1140 | C |
| 1 | AA | 1141 | C |
| 1 | AA | 1142 | G |
| 1 | AA | 1143 | G |
| 1 | AA | 1152 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1158 | C |
| 1 | AA | 1159 | U |
| 1 | AA | 1160 | G |
| 1 | AA | 1167 | A |
| 1 | AA | 1168 | U |
| 1 | AA | 1184 | G |
| 1 | AA | 1196 | A |
| 1 | AA | 1197 | A |
| 1 | AA | 1212 | U |
| 1 | AA | 1213 | A |
| 1 | AA | 1215 | G |
| 1 | AA | 1225 | A |
| 1 | AA | 1227 | A |
| 1 | AA | 1238 | A |
| 1 | AA | 1239 | A |
| 1 | AA | 1240 | U |
| 1 | AA | 1256 | A |
| 1 | AA | 1257 | A |
| 1 | AA | 1260 | G |
| 1 | AA | 1279 | G |
| 1 | AA | 1280 | A |
| 1 | AA | 1286 | U |
| 1 | AA | 1287 | A |
| 1 | AA | 1299 | A |
| 1 | AA | 1300 | G |
| 1 | AA | 1302 | C |
| 1 | AA | 1305 | G |
| 1 | AA | 1317 | C |
| 1 | AA | 1320 | C |
| 1 | AA | 1322 | C |
| 1 | AA | 1323 | G |
| 1 | AA | 1336 | C |
| 1 | AA | 1346 | A |
| 1 | AA | 1353 | G |
| 1 | AA | 1363 | A |
| 1 | AA | 1368 | A |
| 1 | AA | 1370 | G |
| 1 | AA | 1381 | U |
| 1 | AA | 1398 | A |
| 1 | AA | 1429 | A |
| 1 | AA | 1441 | A |
| 1 | AA | 1442 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 1445 | U |
| 1 | AA | 1446 | A |
| 1 | AA | 1450 | U |
| 1 | AA | 1451 | U |
| 1 | AA | 1453 | G |
| 1 | AA | 1454 | G |
| 1 | AA | 1492 | A |
| 1 | AA | 1493 | A |
| 1 | AA | 1497 | G |
| 1 | AA | 1499 | A |
| 1 | AA | 1503 | A |
| 1 | AA | 1505 | G |
| 1 | AA | 1506 | U |
| 1 | AA | 1517 | G |
| 1 | AA | 1529 | G |
| 1 | AA | 1530 | G |
| 1 | BA | 3 | A |
| 1 | BA | 4 | U |
| 1 | BA | 5 | U |
| 1 | BA | 7 | A |
| 1 | BA | 9 | G |
| 1 | BA | 22 | G |
| 1 | BA | 28 | A |
| 1 | BA | 32 | A |
| 1 | BA | 39 | G |
| 1 | BA | 47 | C |
| 1 | BA | 48 | C |
| 1 | BA | 50 | A |
| 1 | BA | 51 | A |
| 1 | BA | 69 | G |
| 1 | BA | 70 | U |
| 1 | BA | 71 | A |
| 1 | BA | 72 | A |
| 1 | BA | 74 | A |
| 1 | BA | 75 | G |
| 1 | BA | 76 | G |
| 1 | BA | 77 | A |
| 1 | BA | 78 | A |
| 1 | BA | 80 | A |
| 1 | BA | 81 | A |
| 1 | BA | 82 | G |
| 1 | BA | 83 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | BA | 84 | U |
| 1 | BA | 85 | U |
| 1 | BA | 87 | C |
| 1 | BA | 88 | U |
| 1 | BA | 94 | G |
| 1 | BA | 95 | C |
| 1 | BA | 108 | G |
| 1 | BA | 119 | A |
| 1 | BA | 121 | U |
| 1 | BA | 122 | G |
| 1 | BA | 128 | G |
| 1 | BA | 130 | A |
| 1 | BA | 131 | A |
| 1 | BA | 137 | U |
| 1 | BA | 142 | G |
| 1 | BA | 144 | G |
| 1 | BA | 158 | G |
| 1 | BA | 159 | G |
| 1 | BA | 163 | C |
| 1 | BA | 168 | G |
| 1 | BA | 173 | U |
| 1 | BA | 182 | A |
| 1 | BA | 183 | C |
| 1 | BA | 201 | G |
| 1 | BA | 204 | G |
| 1 | BA | 209 | U |
| 1 | BA | 210 | C |
| 1 | BA | 211 | G |
| 1 | BA | 212 | G |
| 1 | BA | 245 | U |
| 1 | BA | 247 | G |
| 1 | BA | 251 | G |
| 1 | BA | 262 | A |
| 1 | BA | 266 | G |
| 1 | BA | 267 | C |
| 1 | BA | 289 | G |
| 1 | BA | 321 | A |
| 1 | BA | 328 | C |
| 1 | BA | 329 | A |
| 1 | BA | 330 | C |
| 1 | BA | 332 | G |
| 1 | BA | 346 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | BA | 347 | G |
| 1 | BA | 352 | C |
| 1 | BA | 354 | G |
| 1 | BA | 367 | U |
| 1 | BA | 372 | C |
| 1 | BA | 373 | A |
| 1 | BA | 382 | A |
| 1 | BA | 384 | G |
| 1 | BA | 406 | G |
| 1 | BA | 412 | A |
| 1 | BA | 413 | G |
| 1 | BA | 421 | U |
| 1 | BA | 422 | C |
| 1 | BA | 429 | U |
| 1 | BA | 430 | A |
| 1 | BA | 435 | A |
| 1 | BA | 439 | U |
| 1 | BA | 444 | G |
| 1 | BA | 457 | G |
| 1 | BA | 458 | U |
| 1 | BA | 463 | U |
| 1 | BA | 467 | U |
| 1 | BA | 468 | A |
| 1 | BA | 469 | C |
| 1 | BA | 478 | A |
| 1 | BA | 479 | U |
| 1 | BA | 481 | G |
| 1 | BA | 485 | U |
| 1 | BA | 486 | U |
| 1 | BA | 495 | A |
| 1 | BA | 496 | A |
| 1 | BA | 509 | A |
| 1 | BA | 510 | A |
| 1 | BA | 511 | C |
| 1 | BA | 512 | U |
| 1 | BA | 527 | G7M |
| 1 | BA | 530 | G |
| 1 | BA | 532 | A |
| 1 | BA | 533 | A |
| 1 | BA | 547 | A |
| 1 | BA | 559 | A |
| 1 | BA | 562 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | BA | 564 | C |
| 1 | BA | 568 | G |
| 1 | BA | 572 | A |
| 1 | BA | 573 | A |
| 1 | BA | 576 | C |
| 1 | BA | 577 | G |
| 1 | BA | 631 | C |
| 1 | BA | 632 | U |
| 1 | BA | 649 | A |
| 1 | BA | 650 | G |
| 1 | BA | 653 | U |
| 1 | BA | 665 | A |
| 1 | BA | 682 | G |
| 1 | BA | 723 | U |
| 1 | BA | 724 | G |
| 1 | BA | 733 | G |
| 1 | BA | 753 | A |
| 1 | BA | 755 | G |
| 1 | BA | 777 | A |
| 1 | BA | 793 | U |
| 1 | BA | 794 | A |
| 1 | BA | 815 | A |
| 1 | BA | 817 | C |
| 1 | BA | 827 | U |
| 1 | BA | 828 | U |
| 1 | BA | 841 | C |
| 1 | BA | 842 | U |
| 1 | BA | 843 | U |
| 1 | BA | 844 | G |
| 1 | BA | 845 | A |
| 1 | BA | 846 | G |
| 1 | BA | 858 | G |
| 1 | BA | 887 | G |
| 1 | BA | 913 | A |
| 1 | BA | 914 | A |
| 1 | BA | 926 | G |
| 1 | BA | 932 | C |
| 1 | BA | 934 | C |
| 1 | BA | 942 | G |
| 1 | BA | 960 | U |
| 1 | BA | 969 | A |
| 1 | BA | 975 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | BA | 976 | G |
| 1 | BA | 977 | A |
| 1 | BA | 988 | G |
| 1 | BA | 993 | G |
| 1 | BA | 1004 | A |
| 1 | BA | 1005 | A |
| 1 | BA | 1008 | U |
| 1 | BA | 1009 | U |
| 1 | BA | 1012 | A |
| 1 | BA | 1015 | G |
| 1 | BA | 1017 | U |
| 1 | BA | 1020 | G |
| 1 | BA | 1021 | A |
| 1 | BA | 1023 | U |
| 1 | BA | 1026 | G |
| 1 | BA | 1027 | C |
| 1 | BA | 1028 | C |
| 1 | BA | 1029 | U |
| 1 | BA | 1030 | U |
| 1 | BA | 1031 | C |
| 1 | BA | 1032 | G |
| 1 | BA | 1033 | G |
| 1 | BA | 1034 | G |
| 1 | BA | 1036 | A |
| 1 | BA | 1037 | C |
| 1 | BA | 1041 | G |
| 1 | BA | 1043 | G |
| 1 | BA | 1053 | G |
| 1 | BA | 1054 | C |
| 1 | BA | 1065 | U |
| 1 | BA | 1070 | U |
| 1 | BA | 1086 | U |
| 1 | BA | 1092 | A |
| 1 | BA | 1094 | G |
| 1 | BA | 1095 | U |
| 1 | BA | 1098 | C |
| 1 | BA | 1101 | A |
| 1 | BA | 1108 | G |
| 1 | BA | 1110 | A |
| 1 | BA | 1124 | G |
| 1 | BA | 1133 | G |
| 1 | BA | 1135 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | BA | 1136 | C |
| 1 | BA | 1137 | C |
| 1 | BA | 1139 | G |
| 1 | BA | 1140 | C |
| 1 | BA | 1141 | C |
| 1 | BA | 1142 | G |
| 1 | BA | 1143 | G |
| 1 | BA | 1145 | A |
| 1 | BA | 1152 | A |
| 1 | BA | 1158 | C |
| 1 | BA | 1159 | U |
| 1 | BA | 1160 | G |
| 1 | BA | 1167 | A |
| 1 | BA | 1168 | U |
| 1 | BA | 1183 | U |
| 1 | BA | 1184 | G |
| 1 | BA | 1196 | A |
| 1 | BA | 1197 | A |
| 1 | BA | 1212 | U |
| 1 | BA | 1213 | A |
| 1 | BA | 1214 | C |
| 1 | BA | 1215 | G |
| 1 | BA | 1225 | A |
| 1 | BA | 1227 | A |
| 1 | BA | 1228 | C |
| 1 | BA | 1238 | A |
| 1 | BA | 1239 | A |
| 1 | BA | 1240 | U |
| 1 | BA | 1256 | A |
| 1 | BA | 1257 | A |
| 1 | BA | 1260 | G |
| 1 | BA | 1280 | A |
| 1 | BA | 1286 | U |
| 1 | BA | 1287 | A |
| 1 | BA | 1292 | G |
| 1 | BA | 1293 | C |
| 1 | BA | 1299 | A |
| 1 | BA | 1300 | G |
| 1 | BA | 1302 | C |
| 1 | BA | 1305 | G |
| 1 | BA | 1317 | C |
| 1 | BA | 1320 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | BA | 1322 | C |
| 1 | BA | 1336 | C |
| 1 | BA | 1346 | A |
| 1 | BA | 1353 | G |
| 1 | BA | 1363 | A |
| 1 | BA | 1368 | A |
| 1 | BA | 1370 | G |
| 1 | BA | 1379 | G |
| 1 | BA | 1381 | U |
| 1 | BA | 1398 | A |
| 1 | BA | 1419 | G |
| 1 | BA | 1429 | A |
| 1 | BA | 1441 | A |
| 1 | BA | 1442 | G |
| 1 | BA | 1445 | U |
| 1 | BA | 1446 | A |
| 1 | BA | 1452 | C |
| 1 | BA | 1453 | G |
| 1 | BA | 1454 | G |
| 1 | BA | 1491 | G |
| 1 | BA | 1492 | A |
| 1 | BA | 1493 | A |
| 1 | BA | 1497 | G |
| 1 | BA | 1503 | A |
| 1 | BA | 1505 | G |
| 1 | BA | 1506 | U |
| 1 | BA | 1517 | G |
| 1 | BA | 1529 | G |
| 1 | BA | 1530 | G |
| 1 | BA | 1533 | C |
| 1 | BA | 1534 | A |
| 22 | CA | 7 | G |
| 22 | CA | 10 | A |
| 22 | CA | 14 | A |
| 22 | CA | 15 | G |
| 22 | CA | 34 | U |
| 22 | CA | 42 | A |
| 22 | CA | 46 | G |
| 22 | CA | 58 | G |
| 22 | CA | 63 | A |
| 22 | CA | 71 | A |
| 22 | CA | 74 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | CA | 75 | G |
| 22 | CA | 80 | G |
| 22 | CA | 83 | A |
| 22 | CA | 84 | A |
| 22 | CA | 101 | A |
| 22 | CA | 102 | U |
| 22 | CA | 119 | A |
| 22 | CA | 120 | U |
| 22 | CA | 135 | U |
| 22 | CA | 136 | G |
| 22 | CA | 137 | U |
| 22 | CA | 138 | U |
| 22 | CA | 139 | U |
| 22 | CA | 140 | C |
| 22 | CA | 141 | G |
| 22 | CA | 142 | A |
| 22 | CA | 143 | C |
| 22 | CA | 196 | A |
| 22 | CA | 215 | G |
| 22 | CA | 216 | A |
| 22 | CA | 222 | A |
| 22 | CA | 248 | G |
| 22 | CA | 257 | C |
| 22 | CA | 265 | A |
| 22 | CA | 266 | G |
| 22 | CA | 272 | A |
| 22 | CA | 276 | U |
| 22 | CA | 279 | A |
| 22 | CA | 283 | G |
| 22 | CA | 285 | G |
| 22 | CA | 291 | G |
| 22 | CA | 311 | A |
| 22 | CA | 315 | G |
| 22 | CA | 325 | G |
| 22 | CA | 329 | G |
| 22 | CA | 330 | A |
| 22 | CA | 331 | C |
| 22 | CA | 336 | C |
| 22 | CA | 353 | C |
| 22 | CA | 354 | A |
| 22 | CA | 355 | U |
| 22 | CA | 361 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | CA | 362 | A |
| 22 | CA | 370 | G |
| 22 | CA | 371 | A |
| 22 | CA | 372 | G |
| 22 | CA | 386 | G |
| 22 | CA | 404 | A |
| 22 | CA | 405 | U |
| 22 | CA | 411 | G |
| 22 | CA | 412 | A |
| 22 | CA | 424 | G |
| 22 | CA | 425 | G |
| 22 | CA | 426 | C |
| 22 | CA | 435 | C |
| 22 | CA | 451 | U |
| 22 | CA | 480 | A |
| 22 | CA | 481 | G |
| 22 | CA | 491 | G |
| 22 | CA | 504 | A |
| 22 | CA | 505 | A |
| 22 | CA | 508 | A |
| 22 | CA | 531 | C |
| 22 | CA | 532 | A |
| 22 | CA | 533 | G |
| 22 | CA | 543 | G |
| 22 | CA | 546 | U |
| 22 | CA | 547 | A |
| 22 | CA | 548 | G |
| 22 | CA | 549 | G |
| 22 | CA | 550 | C |
| 22 | CA | 551 | G |
| 22 | CA | 563 | A |
| 22 | CA | 573 | U |
| 22 | CA | 575 | A |
| 22 | CA | 586 | A |
| 22 | CA | 603 | A |
| 22 | CA | 613 | A |
| 22 | CA | 614 | A |
| 22 | CA | 615 | U |
| 22 | CA | 618 | G |
| 22 | CA | 620 | G |
| 22 | CA | 627 | A |
| 22 | CA | 637 | A |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22 | CA | 645 | C |
| 22 | CA | 646 | U |
| 22 | CA | 647 | G |
| 22 | CA | 648 | G |
| 22 | CA | 654 | A |
| 22 | CA | 655 | A |
| 22 | CA | 686 | U |
| 22 | CA | 730 | A |
| 22 | CA | 747 | 5MU |
| 22 | CA | 764 | A |
| 22 | CA | 765 | C |
| 22 | CA | 775 | G |
| 22 | CA | 776 | G |
| 22 | CA | 782 | A |
| 22 | CA | 784 | G |
| 22 | CA | 785 | G |
| 22 | CA | 792 | A |
| 22 | CA | 805 | G |
| 22 | CA | 812 | C |
| 22 | CA | 819 | A |
| 22 | CA | 827 | U |
| 22 | CA | 828 | U |
| 22 | CA | 845 | A |
| 22 | CA | 846 | U |
| 22 | CA | 847 | U |
| 22 | CA | 858 | G |
| 22 | CA | 859 | G |
| 22 | CA | 866 | A |
| 22 | CA | 878 | A |
| 22 | CA | 883 | G |
| 22 | CA | 893 | C |
| 22 | CA | 896 | A |
| 22 | CA | 897 | C |
| 22 | CA | 910 | A |
| 22 | CA | 914 | G |
| 22 | CA | 915 | C |
| 22 | CA | 931 | U |
| 22 | CA | 934 | U |
| 22 | CA | 941 | A |
| 22 | CA | 946 | C |
| 22 | CA | 961 | C |
| 22 | CA | 974 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | CA | 983 | A |
| 22 | CA | 995 | C |
| 22 | CA | 996 | A |
| 22 | CA | 1012 | U |
| 22 | CA | 1013 | C |
| 22 | CA | 1022 | G |
| 22 | CA | 1026 | G |
| 22 | CA | 1033 | U |
| 22 | CA | 1046 | A |
| 22 | CA | 1047 | G |
| 22 | CA | 1053 | C |
| 22 | CA | 1070 | A |
| 22 | CA | 1083 | U |
| 22 | CA | 1084 | A |
| 22 | CA | 1088 | A |
| 22 | CA | 1090 | A |
| 22 | CA | 1110 | G |
| 22 | CA | 1111 | A |
| 22 | CA | 1112 | G |
| 22 | CA | 1122 | G |
| 22 | CA | 1132 | U |
| 22 | CA | 1133 | A |
| 22 | CA | 1135 | C |
| 22 | CA | 1136 | G |
| 22 | CA | 1138 | G |
| 22 | CA | 1142 | A |
| 22 | CA | 1168 | G |
| 22 | CA | 1169 | A |
| 22 | CA | 1171 | G |
| 22 | CA | 1172 | C |
| 22 | CA | 1174 | U |
| 22 | CA | 1175 | A |
| 22 | CA | 1176 | U |
| 22 | CA | 1177 | G |
| 22 | CA | 1179 | G |
| 22 | CA | 1180 | U |
| 22 | CA | 1182 | G |
| 22 | CA | 1186 | G |
| 22 | CA | 1208 | C |
| 22 | CA | 1230 | A |
| 22 | CA | 1231 | U |
| 22 | CA | 1238 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | CA | 1253 | A |
| 22 | CA | 1256 | G |
| 22 | CA | 1266 | G |
| 22 | CA | 1271 | G |
| 22 | CA | 1272 | A |
| 22 | CA | 1273 | U |
| 22 | CA | 1300 | G |
| 22 | CA | 1301 | A |
| 22 | CA | 1365 | A |
| 22 | CA | 1368 | G |
| 22 | CA | 1379 | U |
| 22 | CA | 1380 | G |
| 22 | CA | 1383 | A |
| 22 | CA | 1391 | U |
| 22 | CA | 1395 | A |
| 22 | CA | 1410 | G |
| 22 | CA | 1416 | G |
| 22 | CA | 1417 | C |
| 22 | CA | 1419 | A |
| 22 | CA | 1428 | C |
| 22 | CA | 1452 | G |
| 22 | CA | 1453 | A |
| 22 | CA | 1481 | U |
| 22 | CA | 1482 | G |
| 22 | CA | 1483 | G |
| 22 | CA | 1490 | A |
| 22 | CA | 1493 | C |
| 22 | CA | 1494 | A |
| 22 | CA | 1495 | A |
| 22 | CA | 1497 | U |
| 22 | CA | 1510 | G |
| 22 | CA | 1515 | A |
| 22 | CA | 1523 | U |
| 22 | CA | 1530 | G |
| 22 | CA | 1534 | U |
| 22 | CA | 1535 | A |
| 22 | CA | 1536 | C |
| 22 | CA | 1537 | G |
| 22 | CA | 1540 | G |
| 22 | CA | 1566 | A |
| 22 | CA | 1569 | A |
| 22 | CA | 1578 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | CA | 1581 | G |
| 22 | CA | 1583 | A |
| 22 | CA | 1584 | U |
| 22 | CA | 1585 | C |
| 22 | CA | 1586 | A |
| 22 | CA | 1587 | G |
| 22 | CA | 1606 | C |
| 22 | CA | 1608 | A |
| 22 | CA | 1610 | A |
| 22 | CA | 1647 | U |
| 22 | CA | 1648 | U |
| 22 | CA | 1649 | G |
| 22 | CA | 1674 | G |
| 22 | CA | 1714 | U |
| 22 | CA | 1715 | G |
| 22 | CA | 1725 | U |
| 22 | CA | 1727 | C |
| 22 | CA | 1729 | U |
| 22 | CA | 1730 | C |
| 22 | CA | 1731 | G |
| 22 | CA | 1732 | C |
| 22 | CA | 1738 | G |
| 22 | CA | 1739 | A |
| 22 | CA | 1740 | G |
| 22 | CA | 1744 | A |
| 22 | CA | 1755 | A |
| 22 | CA | 1764 | C |
| 22 | CA | 1773 | A |
| 22 | CA | 1782 | U |
| 22 | CA | 1799 | G |
| 22 | CA | 1800 | C |
| 22 | CA | 1801 | A |
| 22 | CA | 1807 | G |
| 22 | CA | 1808 | A |
| 22 | CA | 1816 | C |
| 22 | CA | 1829 | A |
| 22 | CA | 1858 | A |
| 22 | CA | 1859 | U |
| 22 | CA | 1870 | C |
| 22 | CA | 1871 | A |
| 22 | CA | 1872 | A |
| 22 | CA | 1873 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | CA | 1874 | C |
| 22 | CA | 1876 | A |
| 22 | CA | 1880 | U |
| 22 | CA | 1886 | U |
| 22 | CA | 1906 | G |
| 22 | CA | 1914 | C |
| 22 | CA | 1929 | G |
| 22 | CA | 1930 | G |
| 22 | CA | 1931 | U |
| 22 | CA | 1937 | A |
| 22 | CA | 1938 | A |
| 22 | CA | 1955 | U |
| 22 | CA | 1967 | C |
| 22 | CA | 1970 | A |
| 22 | CA | 1972 | G |
| 22 | CA | 1991 | U |
| 22 | CA | 1993 | U |
| 22 | CA | 1997 | C |
| 22 | CA | 2022 | U |
| 22 | CA | 2023 | C |
| 22 | CA | 2031 | A |
| 22 | CA | 2033 | A |
| 22 | CA | 2043 | C |
| 22 | CA | 2055 | C |
| 22 | CA | 2056 | G |
| 22 | CA | 2060 | A |
| 22 | CA | 2061 | G |
| 22 | CA | 2062 | A |
| 22 | CA | 2069 | G7M |
| 22 | CA | 2072 | C |
| 22 | CA | 2093 | G |
| 22 | CA | 2095 | A |
| 22 | CA | 2101 | A |
| 22 | CA | 2110 | G |
| 22 | CA | 2111 | U |
| 22 | CA | 2112 | G |
| 22 | CA | 2113 | U |
| 22 | CA | 2115 | G |
| 22 | CA | 2116 | G |
| 22 | CA | 2117 | A |
| 22 | CA | 2118 | U |
| 22 | CA | 2119 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | CA | 2123 | G |
| 22 | CA | 2124 | G |
| 22 | CA | 2125 | G |
| 22 | CA | 2126 | A |
| 22 | CA | 2127 | G |
| 22 | CA | 2128 | G |
| 22 | CA | 2131 | U |
| 22 | CA | 2132 | U |
| 22 | CA | 2133 | G |
| 22 | CA | 2137 | U |
| 22 | CA | 2147 | A |
| 22 | CA | 2157 | G |
| 22 | CA | 2158 | A |
| 22 | CA | 2163 | A |
| 22 | CA | 2164 | C |
| 22 | CA | 2165 | C |
| 22 | CA | 2169 | A |
| 22 | CA | 2171 | A |
| 22 | CA | 2172 | U |
| 22 | CA | 2173 | A |
| 22 | CA | 2182 | U |
| 22 | CA | 2183 | A |
| 22 | CA | 2189 | U |
| 22 | CA | 2190 | G |
| 22 | CA | 2198 | A |
| 22 | CA | 2204 | G |
| 22 | CA | 2211 | A |
| 22 | CA | 2212 | A |
| 22 | CA | 2225 | A |
| 22 | CA | 2226 | C |
| 22 | CA | 2238 | G |
| 22 | CA | 2239 | G |
| 22 | CA | 2268 | A |
| 22 | CA | 2273 | A |
| 22 | CA | 2283 | C |
| 22 | CA | 2286 | G |
| 22 | CA | 2287 | A |
| 22 | CA | 2305 | U |
| 22 | CA | 2308 | G |
| 22 | CA | 2311 | A |
| 22 | CA | 2325 | G |
| 22 | CA | 2327 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | CA | 2333 | A |
| 22 | CA | 2335 | A |
| 22 | CA | 2339 | C |
| 22 | CA | 2347 | C |
| 22 | CA | 2361 | G |
| 22 | CA | 2383 | G |
| 22 | CA | 2385 | C |
| 22 | CA | 2402 | U |
| 22 | CA | 2403 | C |
| 22 | CA | 2406 | A |
| 22 | CA | 2423 | U |
| 22 | CA | 2424 | C |
| 22 | CA | 2425 | A |
| 22 | CA | 2426 | A |
| 22 | CA | 2429 | G |
| 22 | CA | 2430 | A |
| 22 | CA | 2431 | U |
| 22 | CA | 2434 | A |
| 22 | CA | 2435 | A |
| 22 | CA | 2441 | U |
| 22 | CA | 2448 | A |
| 22 | CA | 2476 | A |
| 22 | CA | 2491 | U |
| 22 | CA | 2502 | G |
| 22 | CA | 2505 | G |
| 22 | CA | 2518 | A |
| 22 | CA | 2525 | G |
| 22 | CA | 2529 | G |
| 22 | CA | 2547 | A |
| 22 | CA | 2554 | U |
| 22 | CA | 2566 | A |
| 22 | CA | 2567 | G |
| 22 | CA | 2585 | U |
| 22 | CA | 2586 | U |
| 22 | CA | 2603 | G |
| 22 | CA | 2609 | U |
| 22 | CA | 2613 | U |
| 22 | CA | 2629 | U |
| 22 | CA | 2663 | G |
| 22 | CA | 2681 | C |
| 22 | CA | 2682 | A |
| 22 | CA | 2689 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | CA | 2690 | U |
| 22 | CA | 2714 | G |
| 22 | CA | 2718 | G |
| 22 | CA | 2726 | A |
| 22 | CA | 2744 | G |
| 22 | CA | 2748 | A |
| 22 | CA | 2765 | A |
| 22 | CA | 2778 | A |
| 22 | CA | 2791 | G |
| 22 | CA | 2794 | C |
| 22 | CA | 2798 | U |
| 22 | CA | 2799 | A |
| 22 | CA | 2803 | G |
| 22 | CA | 2811 | G |
| 22 | CA | 2820 | A |
| 22 | CA | 2821 | A |
| 22 | CA | 2825 | G |
| 22 | CA | 2867 | G |
| 22 | CA | 2874 | C |
| 22 | CA | 2883 | A |
| 22 | CA | 2884 | U |
| 22 | CA | 2891 | U |
| 22 | CA | 2894 | G |
| 22 | CA | 2903 | U |
| 22 | CA | 2904 | U |
| 23 | CB | 15 | A |
| 23 | CB | 23 | G |
| 23 | CB | 35 | C |
| 23 | CB | 45 | A |
| 23 | CB | 56 | G |
| 23 | CB | 66 | A |
| 23 | CB | 88 | C |
| 23 | CB | 89 | U |
| 23 | CB | 90 | C |
| 23 | CB | 99 | A |
| 23 | CB | 109 | A |
| 53 | DA | 10 | A |
| 53 | DA | 12 | U |
| 53 | DA | 14 | A |
| 53 | DA | 15 | G |
| 53 | DA | 34 | U |
| 53 | DA | 46 | G |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | DA | 58 | G |
| 53 | DA | 63 | A |
| 53 | DA | 71 | A |
| 53 | DA | 74 | A |
| 53 | DA | 75 | G |
| 53 | DA | 80 | G |
| 53 | DA | 101 | A |
| 53 | DA | 102 | U |
| 53 | DA | 119 | A |
| 53 | DA | 120 | U |
| 53 | DA | 135 | U |
| 53 | DA | 136 | G |
| 53 | DA | 137 | U |
| 53 | DA | 138 | U |
| 53 | DA | 139 | U |
| 53 | DA | 140 | C |
| 53 | DA | 141 | G |
| 53 | DA | 142 | A |
| 53 | DA | 196 | A |
| 53 | DA | 216 | A |
| 53 | DA | 221 | A |
| 53 | DA | 222 | A |
| 53 | DA | 248 | G |
| 53 | DA | 257 | C |
| 53 | DA | 266 | G |
| 53 | DA | 272 | A |
| 53 | DA | 276 | U |
| 53 | DA | 277 | G |
| 53 | DA | 279 | A |
| 53 | DA | 283 | G |
| 53 | DA | 285 | G |
| 53 | DA | 291 | G |
| 53 | DA | 302 | C |
| 53 | DA | 311 | A |
| 53 | DA | 315 | G |
| 53 | DA | 325 | G |
| 53 | DA | 329 | G |
| 53 | DA | 330 | A |
| 53 | DA | 331 | C |
| 53 | DA | 353 | C |
| 53 | DA | 355 | U |
| 53 | DA | 358 | U |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53 | DA | 361 | G |
| 53 | DA | 362 | A |
| 53 | DA | 370 | G |
| 53 | DA | 372 | G |
| 53 | DA | 386 | G |
| 53 | DA | 411 | G |
| 53 | DA | 412 | A |
| 53 | DA | 424 | G |
| 53 | DA | 425 | G |
| 53 | DA | 435 | C |
| 53 | DA | 451 | U |
| 53 | DA | 481 | G |
| 53 | DA | 491 | G |
| 53 | DA | 504 | A |
| 53 | DA | 505 | A |
| 53 | DA | 508 | A |
| 53 | DA | 531 | C |
| 53 | DA | 532 | A |
| 53 | DA | 533 | G |
| 53 | DA | 543 | G |
| 53 | DA | 546 | U |
| 53 | DA | 547 | A |
| 53 | DA | 548 | G |
| 53 | DA | 549 | G |
| 53 | DA | 550 | C |
| 53 | DA | 551 | G |
| 53 | DA | 563 | A |
| 53 | DA | 573 | U |
| 53 | DA | 575 | A |
| 53 | DA | 586 | A |
| 53 | DA | 603 | A |
| 53 | DA | 613 | A |
| 53 | DA | 614 | A |
| 53 | DA | 615 | U |
| 53 | DA | 620 | G |
| 53 | DA | 627 | A |
| 53 | DA | 637 | A |
| 53 | DA | 645 | C |
| 53 | DA | 646 | U |
| 53 | DA | 647 | G |
| 53 | DA | 654 | A |
| 53 | DA | 655 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | DA | 686 | U |
| 53 | DA | 730 | A |
| 53 | DA | 747 | 5MU |
| 53 | DA | 764 | A |
| 53 | DA | 765 | C |
| 53 | DA | 775 | G |
| 53 | DA | 776 | G |
| 53 | DA | 782 | A |
| 53 | DA | 784 | G |
| 53 | DA | 785 | G |
| 53 | DA | 790 | U |
| 53 | DA | 792 | A |
| 53 | DA | 805 | G |
| 53 | DA | 812 | C |
| 53 | DA | 827 | U |
| 53 | DA | 828 | U |
| 53 | DA | 845 | A |
| 53 | DA | 846 | U |
| 53 | DA | 847 | U |
| 53 | DA | 858 | G |
| 53 | DA | 859 | G |
| 53 | DA | 866 | A |
| 53 | DA | 878 | A |
| 53 | DA | 885 | C |
| 53 | DA | 893 | C |
| 53 | DA | 896 | A |
| 53 | DA | 897 | C |
| 53 | DA | 910 | A |
| 53 | DA | 914 | G |
| 53 | DA | 915 | C |
| 53 | DA | 931 | U |
| 53 | DA | 934 | U |
| 53 | DA | 946 | C |
| 53 | DA | 961 | C |
| 53 | DA | 974 | G |
| 53 | DA | 983 | A |
| 53 | DA | 996 | A |
| 53 | DA | 1012 | U |
| 53 | DA | 1013 | C |
| 53 | DA | 1022 | G |
| 53 | DA | 1026 | G |
| 53 | DA | 1033 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | DA | 1046 | A |
| 53 | DA | 1047 | G |
| 53 | DA | 1070 | A |
| 53 | DA | 1083 | U |
| 53 | DA | 1084 | A |
| 53 | DA | 1088 | A |
| 53 | DA | 1090 | A |
| 53 | DA | 1112 | G |
| 53 | DA | 1130 | U |
| 53 | DA | 1132 | U |
| 53 | DA | 1133 | A |
| 53 | DA | 1135 | C |
| 53 | DA | 1136 | G |
| 53 | DA | 1138 | G |
| 53 | DA | 1142 | A |
| 53 | DA | 1168 | G |
| 53 | DA | 1171 | G |
| 53 | DA | 1172 | C |
| 53 | DA | 1174 | U |
| 53 | DA | 1175 | A |
| 53 | DA | 1176 | U |
| 53 | DA | 1177 | G |
| 53 | DA | 1182 | G |
| 53 | DA | 1238 | G |
| 53 | DA | 1253 | A |
| 53 | DA | 1256 | G |
| 53 | DA | 1271 | G |
| 53 | DA | 1272 | A |
| 53 | DA | 1273 | U |
| 53 | DA | 1300 | G |
| 53 | DA | 1301 | A |
| 53 | DA | 1352 | U |
| 53 | DA | 1365 | A |
| 53 | DA | 1379 | U |
| 53 | DA | 1383 | A |
| 53 | DA | 1410 | G |
| 53 | DA | 1416 | G |
| 53 | DA | 1417 | C |
| 53 | DA | 1419 | A |
| 53 | DA | 1428 | C |
| 53 | DA | 1452 | G |
| 53 | DA | 1453 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | DA | 1482 | G |
| 53 | DA | 1490 | A |
| 53 | DA | 1493 | C |
| 53 | DA | 1494 | A |
| 53 | DA | 1495 | A |
| 53 | DA | 1497 | U |
| 53 | DA | 1510 | G |
| 53 | DA | 1515 | A |
| 53 | DA | 1523 | U |
| 53 | DA | 1532 | A |
| 53 | DA | 1535 | A |
| 53 | DA | 1536 | C |
| 53 | DA | 1537 | G |
| 53 | DA | 1540 | G |
| 53 | DA | 1566 | A |
| 53 | DA | 1569 | A |
| 53 | DA | 1578 | U |
| 53 | DA | 1581 | G |
| 53 | DA | 1583 | A |
| 53 | DA | 1584 | U |
| 53 | DA | 1585 | C |
| 53 | DA | 1606 | C |
| 53 | DA | 1608 | A |
| 53 | DA | 1647 | U |
| 53 | DA | 1648 | U |
| 53 | DA | 1649 | G |
| 53 | DA | 1674 | G |
| 53 | DA | 1714 | U |
| 53 | DA | 1715 | G |
| 53 | DA | 1725 | U |
| 53 | DA | 1727 | C |
| 53 | DA | 1729 | U |
| 53 | DA | 1730 | C |
| 53 | DA | 1731 | G |
| 53 | DA | 1732 | C |
| 53 | DA | 1738 | G |
| 53 | DA | 1739 | A |
| 53 | DA | 1740 | G |
| 53 | DA | 1744 | A |
| 53 | DA | 1755 | A |
| 53 | DA | 1764 | C |
| 53 | DA | 1773 | A |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | DA | 1782 | U |
| 53 | DA | 1800 | C |
| 53 | DA | 1801 | A |
| 53 | DA | 1808 | A |
| 53 | DA | 1816 | C |
| 53 | DA | 1829 | A |
| 53 | DA | 1858 | A |
| 53 | DA | 1859 | U |
| 53 | DA | 1870 | C |
| 53 | DA | 1871 | A |
| 53 | DA | 1872 | A |
| 53 | DA | 1873 | G |
| 53 | DA | 1874 | C |
| 53 | DA | 1876 | A |
| 53 | DA | 1880 | U |
| 53 | DA | 1886 | U |
| 53 | DA | 1906 | G |
| 53 | DA | 1907 | G |
| 53 | DA | 1913 | A |
| 53 | DA | 1914 | C |
| 53 | DA | 1929 | G |
| 53 | DA | 1930 | G |
| 53 | DA | 1931 | U |
| 53 | DA | 1937 | A |
| 53 | DA | 1938 | A |
| 53 | DA | 1955 | U |
| 53 | DA | 1967 | C |
| 53 | DA | 1970 | A |
| 53 | DA | 1972 | G |
| 53 | DA | 1991 | U |
| 53 | DA | 1993 | U |
| 53 | DA | 1997 | C |
| 53 | DA | 2023 | C |
| 53 | DA | 2031 | A |
| 53 | DA | 2033 | A |
| 53 | DA | 2043 | C |
| 53 | DA | 2055 | C |
| 53 | DA | 2056 | G |
| 53 | DA | 2060 | A |
| 53 | DA | 2061 | G |
| 53 | DA | 2062 | A |
| 53 | DA | 2069 | G7M |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | DA | 2085 | U |
| 53 | DA | 2093 | G |
| 53 | DA | 2097 | A |
| 53 | DA | 2101 | A |
| 53 | DA | 2105 | U |
| 53 | DA | 2108 | A |
| 53 | DA | 2111 | U |
| 53 | DA | 2112 | G |
| 53 | DA | 2113 | U |
| 53 | DA | 2115 | G |
| 53 | DA | 2116 | G |
| 53 | DA | 2117 | A |
| 53 | DA | 2118 | U |
| 53 | DA | 2119 | A |
| 53 | DA | 2123 | G |
| 53 | DA | 2126 | A |
| 53 | DA | 2127 | G |
| 53 | DA | 2128 | G |
| 53 | DA | 2131 | U |
| 53 | DA | 2132 | U |
| 53 | DA | 2133 | G |
| 53 | DA | 2134 | A |
| 53 | DA | 2136 | G |
| 53 | DA | 2137 | U |
| 53 | DA | 2145 | C |
| 53 | DA | 2146 | C |
| 53 | DA | 2147 | A |
| 53 | DA | 2148 | G |
| 53 | DA | 2149 | U |
| 53 | DA | 2159 | G |
| 53 | DA | 2160 | C |
| 53 | DA | 2161 | C |
| 53 | DA | 2162 | G |
| 53 | DA | 2163 | A |
| 53 | DA | 2164 | C |
| 53 | DA | 2165 | C |
| 53 | DA | 2167 | U |
| 53 | DA | 2168 | G |
| 53 | DA | 2169 | A |
| 53 | DA | 2170 | A |
| 53 | DA | 2171 | A |
| 53 | DA | 2172 | U |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | DA | 2173 | A |
| 53 | DA | 2177 | C |
| 53 | DA | 2178 | C |
| 53 | DA | 2179 | C |
| 53 | DA | 2181 | U |
| 53 | DA | 2185 | U |
| 53 | DA | 2187 | U |
| 53 | DA | 2188 | U |
| 53 | DA | 2190 | G |
| 53 | DA | 2198 | A |
| 53 | DA | 2204 | G |
| 53 | DA | 2211 | A |
| 53 | DA | 2225 | A |
| 53 | DA | 2238 | G |
| 53 | DA | 2239 | G |
| 53 | DA | 2268 | A |
| 53 | DA | 2283 | C |
| 53 | DA | 2286 | G |
| 53 | DA | 2287 | A |
| 53 | DA | 2305 | U |
| 53 | DA | 2308 | G |
| 53 | DA | 2325 | G |
| 53 | DA | 2327 | A |
| 53 | DA | 2333 | A |
| 53 | DA | 2335 | A |
| 53 | DA | 2339 | C |
| 53 | DA | 2347 | C |
| 53 | DA | 2383 | G |
| 53 | DA | 2385 | C |
| 53 | DA | 2406 | A |
| 53 | DA | 2424 | C |
| 53 | DA | 2425 | A |
| 53 | DA | 2434 | A |
| 53 | DA | 2435 | A |
| 53 | DA | 2441 | U |
| 53 | DA | 2448 | A |
| 53 | DA | 2476 | A |
| 53 | DA | 2491 | U |
| 53 | DA | 2502 | G |
| 53 | DA | 2505 | G |
| 53 | DA | 2518 | A |
| 53 | DA | 2525 | G |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 53 | DA | 2529 | G |
| 53 | DA | 2547 | A |
| 53 | DA | 2554 | U |
| 53 | DA | 2566 | A |
| 53 | DA | 2567 | G |
| 53 | DA | 2573 | C |
| 53 | DA | 2585 | U |
| 53 | DA | 2586 | U |
| 53 | DA | 2603 | G |
| 53 | DA | 2609 | U |
| 53 | DA | 2613 | U |
| 53 | DA | 2629 | U |
| 53 | DA | 2663 | G |
| 53 | DA | 2682 | A |
| 53 | DA | 2689 | U |
| 53 | DA | 2690 | U |
| 53 | DA | 2714 | G |
| 53 | DA | 2726 | A |
| 53 | DA | 2744 | G |
| 53 | DA | 2748 | A |
| 53 | DA | 2765 | A |
| 53 | DA | 2778 | A |
| 53 | DA | 2791 | G |
| 53 | DA | 2798 | U |
| 53 | DA | 2799 | A |
| 53 | DA | 2803 | G |
| 53 | DA | 2811 | G |
| 53 | DA | 2820 | A |
| 53 | DA | 2821 | A |
| 53 | DA | 2825 | G |
| 53 | DA | 2867 | G |
| 53 | DA | 2874 | C |
| 53 | DA | 2883 | A |
| 53 | DA | 2891 | U |
| 53 | DA | 2894 | G |
| 23 | DB | 25 | U |
| 23 | DB | 35 | C |
| 23 | DB | 45 | A |
| 23 | DB | 56 | G |
| 23 | DB | 66 | A |
| 23 | DB | 89 | U |
| 23 | DB | 90 | C |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23 | DB | 109 | A |

All (77) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | AA | 4 | U |
| 1 | AA | 209 | U |
| 1 | AA | 412 | A |
| 1 | AA | 429 | U |
| 1 | AA | 653 | U |
| 1 | AA | 793 | U |
| 1 | AA | 1024 | G |
| 1 | AA | 1031 | C |
| 1 | AA | 1211 | U |
| 1 | BA | 4 | U |
| 1 | BA | 83 | C |
| 1 | BA | 209 | U |
| 1 | BA | 429 | U |
| 1 | BA | 653 | U |
| 1 | BA | 793 | U |
| 1 | BA | 1028 | C |
| 1 | BA | 1183 | U |
| 1 | BA | 1211 | U |
| 1 | BA | 1493 | A |
| 22 | CA | 199 | A |
| 22 | CA | 271 | G |
| 22 | CA | 335 | C |
| 22 | CA | 404 | A |
| 22 | CA | 627 | A |
| 22 | CA | 645 | C |
| 22 | CA | 647 | G |
| 22 | CA | 764 | A |
| 22 | CA | 776 | G |
| 22 | CA | 784 | G |
| 22 | CA | 846 | U |
| 22 | CA | 960 | A |
| 22 | CA | 984 | A |
| 22 | CA | 1128 | G |
| 22 | CA | 1142 | A |
| 22 | CA | 1379 | U |
| 22 | CA | 1647 | U |
| 22 | CA | 1730 | C |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 22 | CA | 1738 | G |
| 22 | CA | 2118 | U |
| 22 | CA | 2146 | C |
| 22 | CA | 2162 | G |
| 22 | CA | 2225 | A |
| 22 | CA | 2286 | G |
| 22 | CA | 2324 | U |
| 22 | CA | 2326 | C |
| 22 | CA | 2406 | A |
| 22 | CA | 2425 | A |
| 22 | CA | 2585 | U |
| 22 | CA | 2680 | U |
| 22 | CA | 2873 | A |
| 22 | CA | 2903 | U |
| 53 | DA | 199 | A |
| 53 | DA | 627 | A |
| 53 | DA | 645 | C |
| 53 | DA | 764 | A |
| 53 | DA | 776 | G |
| 53 | DA | 784 | G |
| 53 | DA | 846 | U |
| 53 | DA | 859 | G |
| 53 | DA | 984 | A |
| 53 | DA | 1046 | A |
| 53 | DA | 1128 | G |
| 53 | DA | 1142 | A |
| 53 | DA | 1253 | A |
| 53 | DA | 1494 | A |
| 53 | DA | 1647 | U |
| 53 | DA | 1730 | C |
| 53 | DA | 1738 | G |
| 53 | DA | 1929 | G |
| 53 | DA | 2118 | U |
| 53 | DA | 2127 | G |
| 53 | DA | 2130 | U |
| 53 | DA | 2158 | A |
| 53 | DA | 2324 | U |
| 53 | DA | 2406 | A |
| 53 | DA | 2585 | U |
| 53 | DA | 2873 | A |

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

75 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 1 | 2MG | AA | 1207 | 1 | 17,26,27 | 1.18 | 2 (11%) | 21,38,41 | 2.39 | 9 (42%) |
| 1 | 4OC | AA | 1402 | 1 | 13,23,24 | 0.46 | 0 | 18,32,35 | 1.61 | 1 (5%) |
| 1 | 5MC | AA | 1407 | 1 | 13,22,23 | 1.53 | 1 (7%) | 15,32,35 | 1.00 | 1 (6%) |
| 1 | UR3 | AA | 1498 | 1 | 12,22,23 | 0.60 | 0 | 16,32,35 | 0.78 | 0 |
| 1 | 2MG | AA | 1516 | 1 | 17,26,27 | 1.09 | 2 (11%) | 21,38,41 | 2.21 | 7 (33%) |
| 1 | MA6 | AA | 1518 | 1 | 16,26,27 | 0.99 | 1 (6%) | 18,38,41 | 2.08 | 3 (16%) |
| 1 | MA6 | AA | 1519 | 1 | 16,26,27 | 0.95 | 1 (6%) | 18,38,41 | 2.62 | 5 (27%) |
| 1 | PSU | AA | 516 | 1,56 | 13,21,22 | 1.12 | 1 (7%) | 18,30,33 | 3.51 | 5 (27%) |
| 1 | G7M | AA | 527 | 1 | 17,26,27 | 1.10 | 1 (5%) | 19,39,42 | 2.19 | 6 (31%) |
| 1 | 2MG | AA | 966 | 1 | 17,26,27 | 1.29 | 2 (11%) | 21,38,41 | 2.26 | 7 (33%) |
| 1 | 5MC | AA | 967 | 1 | 13,22,23 | 1.26 | 1 (7%) | 15,32,35 | 1.30 | 2 (13%) |
| 12 | D2T | AL | 89 | 12 | 4,9,10 | 0.58 | 0 | 4,11,13 | 1.09 | 0 |
| 1 | 2MG | BA | 1207 | 1 | 17,26,27 | 1.30 | 2 (11%) | 21,38,41 | 2.47 | 10 (47%) |
| 1 | 4OC | BA | 1402 | 1 | 13,23,24 | 0.58 | 0 | 18,32,35 | 1.08 | 2 (11%) |
| 1 | 5MC | BA | 1407 | 1 | 13,22,23 | 1.52 | 1 (7%) | 15,32,35 | 0.95 | 1 (6%) |
| 1 | UR3 | BA | 1498 | 1 | 12,22,23 | 0.82 | 1 (8%) | 16,32,35 | 0.73 | 0 |
| 1 | 2MG | BA | 1516 | 1 | 17,26,27 | 1.29 | 2 (11%) | 21,38,41 | 2.30 | 6 (28%) |
| 1 | MA6 | BA | 1518 | 1 | 16,26,27 | 1.00 | 1 (6%) | 18,38,41 | 2.38 | 3 (16%) |
| 1 | MA6 | BA | 1519 | 1 | 16,26,27 | 1.03 | 1 (6%) | 18,38,41 | 2.77 | 6 (33%) |
| 1 | PSU | BA | 516 | 1 | 13,21,22 | 0.83 | 1 (7%) | 18,30,33 | 3.70 | 5 (27%) |
| 1 | G7M | BA | 527 | 1 | 17,26,27 | 1.12 | 1 (5%) | 19,39,42 | 1.90 | 4 (21%) |
| 1 | 2MG | BA | 966 | 1 | 17,26,27 | 1.27 | 2 (11%) | 21,38,41 | 2.23 | 7 (33%) |
| 1 | 5MC | BA | 967 | 1 | 13,22,23 | 1.40 | 1 (7%) | 15,32,35 | 0.96 | 1 (6%) |
| 12 | D2T | BL | 89 | 12 | 4,9,10 | 0.62 | 0 | 4,11,13 | 1.41 | 1 (25%) |
| 22 | 6MZ | CA | 1618 | 22 | 16,25,26 | 1.10 | 1 (6%) | 17,36,39 | 3.07 | 5 (29%) |
| 22 | 2MG | CA | 1835 | 22 | 17,26,27 | 1.25 | 2 (11%) | 21,38,41 | 2.27 | 8 (38%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | PSU | CA | 1911 | 22 | 13,21,22 | 1.08 | 1 (7%) | 18,30,33 | 3.57 | 5 (27%) |
| 22 | 3TD | CA | 1915 | 22 | 14,22,23 | 1.86 | 3 (21%) | 18,32,35 | 1.92 | 4 (22%) |
| 22 | PSU | CA | 1917 | 22 | 13,21,22 | 1.11 | 1 (7%) | 18,30,33 | 3.71 | 5 (27%) |
| 22 | 5MU | CA | 1939 | 22 | 12,22,23 | 0.45 | 0 | 14,32,35 | 2.38 | 2 (14%) |
| 22 | 5MC | CA | 1962 | 22 | 13,22,23 | 1.42 | 1 (7%) | 15,32,35 | 1.11 | 1 (6%) |
| 22 | 6MZ | CA | 2030 | 22 | 16,25,26 | 1.03 | 1 (6%) | 17,36,39 | 3.27 | 5 (29%) |
| 22 | G7M | CA | 2069 | 22 | 17,26,27 | 1.16 | 1 (5%) | 19,39,42 | 1.87 | 3 (15%) |
| 22 | OMG | CA | 2251 | 22 | 17,26,27 | 1.32 | 2 (11%) | 21,38,41 | 1.97 | 7 (33%) |
| 22 | 2MG | CA | 2445 | 22 | 17,26,27 | 1.35 | 2 (11%) | 21,38,41 | 2.39 | 7 (33%) |
| 22 | PSU | CA | 2457 | 22 | 13,21,22 | 0.98 | 1 (7%) | 18,30,33 | 3.45 | 5 (27%) |
| 22 | OMC | CA | 2498 | 56,22 | 13,22,23 | 0.42 | 0 | 20,31,34 | 1.10 | 2 (10%) |
| 22 | 2MA | CA | 2503 | 22 | 16,25,26 | 1.84 | 3 (18%) | 18,37,40 | 2.20 | 3 (16%) |
| 22 | PSU | CA | 2504 | 22 | 13,21,22 | 0.95 | 1 (7%) | 18,30,33 | 3.78 | 5 (27%) |
| 22 | OMU | CA | 2552 | 22 | 12,22,23 | 0.43 | 0 | 19,31,34 | 1.63 | 1 (5%) |
| 22 | PSU | CA | 2580 | 22 | 13,21,22 | 1.04 | 1 (7%) | 18,30,33 | 3.60 | 5 (27%) |
| 22 | PSU | CA | 2605 | 22 | 13,21,22 | 0.92 | 1 (7%) | 18,30,33 | 3.63 | 6 (33%) |
| 22 | 1MG | CA | 745 | 22 | 16,26,27 | 1.52 | 2 (12%) | 19,39,42 | 1.11 | 2 (10%) |
| 22 | PSU | CA | 746 | 56,22 | 13,21,22 | 0.98 | 1 (7%) | 18,30,33 | 3.27 | 5 (27%) |
| 22 | 5MU | CA | 747 | 22 | 12,22,23 | 0.48 | 0 | 14,32,35 | 2.00 | 2 (14%) |
| 22 | PSU | CA | 955 | 22 | 13,21,22 | 1.13 | 2 (15%) | 18,30,33 | 3.64 | 5 (27%) |
| 34 | 4D4 | CN | 81 | 34 | 6,11,12 | 1.26 | 1 (16%) | 5,13,15 | 0.83 | 0 |
| 53 | 6MZ | DA | 1618 | 53 | 16,25,26 | 1.01 | 1 (6%) | 17,36,39 | 2.84 | 5 (29%) |
| 53 | 2MG | DA | 1835 | 53 | 17,26,27 | 0.98 | 2 (11%) | 21,38,41 | 2.44 | 8 (38%) |
| 53 | PSU | DA | 1911 | 53 | 13,21,22 | 1.10 | 1 (7%) | 18,30,33 | 3.54 | 5 (27%) |
| 53 | 3TD | DA | 1915 | 53 | 14,22,23 | 1.44 | 3 (21%) | 18,32,35 | 1.69 | 4 (22%) |
| 53 | PSU | DA | 1917 | 53 | 13,21,22 | 1.32 | 2 (15%) | 18,30,33 | 3.66 | 6 (33%) |
| 53 | 5MU | DA | 1939 | 53 | 12,22,23 | 0.55 | 0 | 14,32,35 | 2.64 | 2 (14%) |
| 53 | 5MC | DA | 1962 | 53 | 13,22,23 | 1.26 | 1 (7%) | 15,32,35 | 0.89 | 1 (6%) |
| 53 | 6MZ | DA | 2030 | 53 | 16,25,26 | 0.74 | 0 | 17,36,39 | 3.40 | 5 (29%) |
| 53 | G7M | DA | 2069 | 53 | 17,26,27 | 0.89 | 1 (5%) | 19,39,42 | 2.03 | 4 (21%) |
| 53 | OMG | DA | 2251 | 53 | 17,26,27 | 1.19 | 2 (11%) | 21,38,41 | 1.82 | 6 (28%) |
| 53 | 2MG | DA | 2445 | 53 | 17,26,27 | 1.41 | 2 (11%) | 21,38,41 | 2.49 | 8 (38%) |
| 53 | H2U | DA | 2449 | 53 | 17,21,22 | 1.33 | 2 (11%) | 23,30,33 | 2.38 | 7 (30%) |
| 53 | PSU | DA | 2457 | 53 | 13,21,22 | 1.24 | 1 (7%) | 18,30,33 | 4.28 | 5 (27%) |
| 53 | OMC | DA | 2498 | 56,53 | 13,22,23 | 0.86 | 1 (7%) | 20,31,34 | 1.27 | 2 (10%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|--------|-------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 53 | 2MA | DA | 2503 | 56,53 | 16,25,26 | 1.34 | 3 (18%) | 18,37,40 | 2.30 | 3 (16%) |
| 53 | PSU | DA | 2504 | 53 | 13,21,22 | 1.40 | 2 (15%) | 18,30,33 | 4.01 | 4 (22%) |
| 53 | OMU | DA | 2552 | 53 | 12,22,23 | 0.62 | 0 | 19,31,34 | 1.60 | 1 (5%) |
| 53 | PSU | DA | 2580 | 53 | 13,21,22 | 1.15 | 1 (7%) | 18,30,33 | 4.55 | 5 (27%) |
| 53 | PSU | DA | 2604 | 53 | 13,21,22 | 1.54 | 2 (15%) | 18,30,33 | 4.18 | 5 (27%) |
| 53 | PSU | DA | 2605 | 53 | 13,21,22 | 1.43 | 2 (15%) | 18,30,33 | 3.70 | 5 (27%) |
| 53 | 1MG | DA | 745 | 53 | 16,26,27 | 1.39 | 2 (12%) | 19,39,42 | 1.40 | 2 (10%) |
| 53 | PSU | DA | 746 | 56,53 | 13,21,22 | 1.54 | 4 (30%) | 18,30,33 | 3.02 | 5 (27%) |
| 53 | 5MU | DA | 747 | 53 | 12,22,23 | 0.49 | 0 | 14,32,35 | 2.13 | 2 (14%) |
| 53 | PSU | DA | 955 | 53 | 13,21,22 | 1.47 | 3 (23%) | 18,30,33 | 4.03 | 3 (16%) |
| 54 | MEQ | DD | 150[A] | 54 | 8,9,10 | 0.86 | 0 | 7,10,12 | 1.26 | 1 (14%) |
| 54 | MEQ | DD | 150[B] | 54 | 8,9,10 | 1.14 | 1 (12%) | 7,10,12 | 0.90 | 0 |
| 34 | 4D4 | DN | 81[A] | - | 6,11,12 | 1.37 | 1 (16%) | 5,13,15 | 1.10 | 0 |
| 34 | 4D4 | DN | 81[B] | - | 6,11,12 | 1.20 | 0 | 5,13,15 | 1.17 | 1 (20%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 1 | 2MG | AA | 1207 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 4OC | AA | 1402 | 1 | - | 0/7/29/30 | 0/2/2/2 |
| 1 | 5MC | AA | 1407 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | UR3 | AA | 1498 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | 2MG | AA | 1516 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | MA6 | AA | 1518 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | MA6 | AA | 1519 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | PSU | AA | 516 | 1,56 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | G7M | AA | 527 | 1 | - | 0/3/25/26 | 0/3/3/3 |
| 1 | 2MG | AA | 966 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 5MC | AA | 967 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 12 | D2T | AL | 89 | 12 | - | 0/2/12/14 | 0/0/0/0 |
| 1 | 2MG | BA | 1207 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 4OC | BA | 1402 | 1 | - | 0/7/29/30 | 0/2/2/2 |
| 1 | 5MC | BA | 1407 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | UR3 | BA | 1498 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | 2MG | BA | 1516 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | MA6 | BA | 1518 | 1 | - | 0/7/29/30 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|-------|---------|-----------|---------|
| 1 | MA6 | BA | 1519 | 1 | - | 0/7/29/30 | 0/3/3/3 |
| 1 | PSU | BA | 516 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | G7M | BA | 527 | 1 | - | 0/3/25/26 | 0/3/3/3 |
| 1 | 2MG | BA | 966 | 1 | - | 0/5/27/28 | 0/3/3/3 |
| 1 | 5MC | BA | 967 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 12 | D2T | BL | 89 | 12 | - | 0/2/12/14 | 0/0/0/0 |
| 22 | 6MZ | CA | 1618 | 22 | - | 0/5/27/28 | 0/3/3/3 |
| 22 | 2MG | CA | 1835 | 22 | - | 0/5/27/28 | 0/3/3/3 |
| 22 | PSU | CA | 1911 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 3TD | CA | 1915 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | PSU | CA | 1917 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 5MU | CA | 1939 | 22 | - | 0/3/25/26 | 0/2/2/2 |
| 22 | 5MC | CA | 1962 | 22 | - | 0/3/25/26 | 0/2/2/2 |
| 22 | 6MZ | CA | 2030 | 22 | - | 0/5/27/28 | 0/3/3/3 |
| 22 | G7M | CA | 2069 | 22 | - | 0/3/25/26 | 0/3/3/3 |
| 22 | OMG | CA | 2251 | 22 | - | 0/5/27/28 | 0/3/3/3 |
| 22 | 2MG | CA | 2445 | 22 | - | 0/5/27/28 | 0/3/3/3 |
| 22 | PSU | CA | 2457 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | OMC | CA | 2498 | 56,22 | - | 0/5/27/28 | 0/2/2/2 |
| 22 | 2MA | CA | 2503 | 22 | - | 0/3/25/26 | 0/3/3/3 |
| 22 | PSU | CA | 2504 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | OMU | CA | 2552 | 22 | - | 0/5/27/28 | 0/2/2/2 |
| 22 | PSU | CA | 2580 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | PSU | CA | 2605 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 1MG | CA | 745 | 22 | - | 0/3/25/26 | 0/3/3/3 |
| 22 | PSU | CA | 746 | 56,22 | - | 0/7/25/26 | 0/2/2/2 |
| 22 | 5MU | CA | 747 | 22 | - | 0/3/25/26 | 0/2/2/2 |
| 22 | PSU | CA | 955 | 22 | - | 0/7/25/26 | 0/2/2/2 |
| 34 | 4D4 | CN | 81 | 34 | - | 0/8/12/14 | 0/0/0/0 |
| 53 | 6MZ | DA | 1618 | 53 | - | 0/5/27/28 | 0/3/3/3 |
| 53 | 2MG | DA | 1835 | 53 | - | 0/5/27/28 | 0/3/3/3 |
| 53 | PSU | DA | 1911 | 53 | - | 0/7/25/26 | 0/2/2/2 |
| 53 | 3TD | DA | 1915 | 53 | - | 0/7/25/26 | 0/2/2/2 |
| 53 | PSU | DA | 1917 | 53 | - | 0/7/25/26 | 0/2/2/2 |
| 53 | 5MU | DA | 1939 | 53 | - | 0/3/25/26 | 0/2/2/2 |
| 53 | 5MC | DA | 1962 | 53 | - | 0/3/25/26 | 0/2/2/2 |
| 53 | 6MZ | DA | 2030 | 53 | - | 0/5/27/28 | 0/3/3/3 |
| 53 | G7M | DA | 2069 | 53 | - | 0/3/25/26 | 0/3/3/3 |
| 53 | OMG | DA | 2251 | 53 | - | 0/5/27/28 | 0/3/3/3 |
| 53 | 2MG | DA | 2445 | 53 | - | 0/5/27/28 | 0/3/3/3 |
| 53 | H2U | DA | 2449 | 53 | - | 0/7/38/39 | 0/2/2/2 |
| 53 | PSU | DA | 2457 | 53 | - | 0/7/25/26 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|--------|-------|---------|-----------|---------|
| 53 | OMC | DA | 2498 | 56,53 | - | 0/5/27/28 | 0/2/2/2 |
| 53 | 2MA | DA | 2503 | 56,53 | - | 0/3/25/26 | 0/3/3/3 |
| 53 | PSU | DA | 2504 | 53 | - | 0/7/25/26 | 0/2/2/2 |
| 53 | OMU | DA | 2552 | 53 | - | 0/5/27/28 | 0/2/2/2 |
| 53 | PSU | DA | 2580 | 53 | - | 0/7/25/26 | 0/2/2/2 |
| 53 | PSU | DA | 2604 | 53 | - | 0/7/25/26 | 0/2/2/2 |
| 53 | PSU | DA | 2605 | 53 | - | 0/7/25/26 | 0/2/2/2 |
| 53 | 1MG | DA | 745 | 53 | - | 0/3/25/26 | 0/3/3/3 |
| 53 | PSU | DA | 746 | 56,53 | - | 0/7/25/26 | 0/2/2/2 |
| 53 | 5MU | DA | 747 | 53 | - | 0/3/25/26 | 0/2/2/2 |
| 53 | PSU | DA | 955 | 53 | - | 0/7/25/26 | 0/2/2/2 |
| 54 | MEQ | DD | 150[A] | 54 | - | 0/7/9/11 | 0/0/0/0 |
| 54 | MEQ | DD | 150[B] | 54 | - | 1/7/9/11 | 0/0/0/0 |
| 34 | 4D4 | DN | 81[A] | - | - | 0/8/12/14 | 0/0/0/0 |
| 34 | 4D4 | DN | 81[B] | - | - | 0/8/12/14 | 0/0/0/0 |

All (93) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-------|------|---------|-------|-------------|----------|
| 22 | CA | 1915 | 3TD | C5-C1' | -5.48 | 1.47 | 1.52 |
| 53 | DA | 2604 | PSU | C5-C1' | -3.70 | 1.49 | 1.52 |
| 53 | DA | 2605 | PSU | C5-C1' | -3.64 | 1.49 | 1.52 |
| 53 | DA | 1915 | 3TD | C5-C1' | -3.37 | 1.49 | 1.52 |
| 53 | DA | 746 | PSU | C5-C1' | -3.21 | 1.49 | 1.52 |
| 53 | DA | 746 | PSU | C2'-C1' | -3.11 | 1.50 | 1.53 |
| 53 | DA | 1917 | PSU | C5-C1' | -2.70 | 1.49 | 1.52 |
| 53 | DA | 955 | PSU | C2'-C1' | -2.61 | 1.51 | 1.53 |
| 53 | DA | 1915 | 3TD | C4-N3 | -2.47 | 1.34 | 1.38 |
| 53 | DA | 955 | PSU | C5-C1' | -2.41 | 1.50 | 1.52 |
| 34 | DN | 81[A] | 4D4 | CD-NE | -2.38 | 1.42 | 1.47 |
| 53 | DA | 2449 | H2U | C4-N3 | -2.37 | 1.33 | 1.37 |
| 53 | DA | 746 | PSU | O4'-C1' | -2.25 | 1.40 | 1.44 |
| 22 | CA | 1915 | 3TD | C4-N3 | -2.24 | 1.35 | 1.38 |
| 53 | DA | 2498 | OMC | C6-N1 | -2.18 | 1.32 | 1.35 |
| 34 | CN | 81 | 4D4 | CD-NE | -2.08 | 1.42 | 1.47 |
| 53 | DA | 2504 | PSU | C5-C1' | -2.06 | 1.50 | 1.52 |
| 53 | DA | 2503 | 2MA | C5-C4 | 2.02 | 1.45 | 1.40 |
| 53 | DA | 1835 | 2MG | C5-C4 | 2.03 | 1.45 | 1.40 |
| 53 | DA | 746 | PSU | C4-N3 | 2.08 | 1.37 | 1.33 |
| 1 | BA | 516 | PSU | C4-N3 | 2.20 | 1.37 | 1.33 |
| 22 | CA | 955 | PSU | C5-C1' | 2.41 | 1.54 | 1.52 |
| 1 | BA | 1498 | UR3 | C4-N3 | 2.42 | 1.41 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|--------|------|-------------|----------|
| 54 | DD | 150[B] | MEQ | OE1-CD | 2.45 | 1.28 | 1.23 |
| 1 | AA | 1519 | MA6 | C5-C4 | 2.53 | 1.46 | 1.40 |
| 22 | CA | 746 | PSU | C4-N3 | 2.56 | 1.37 | 1.33 |
| 53 | DA | 2605 | PSU | C4-N3 | 2.67 | 1.38 | 1.33 |
| 53 | DA | 2604 | PSU | C4-N3 | 2.67 | 1.38 | 1.33 |
| 22 | CA | 2605 | PSU | C4-N3 | 2.68 | 1.38 | 1.33 |
| 53 | DA | 1915 | 3TD | C10-N3 | 2.68 | 1.53 | 1.47 |
| 1 | BA | 1519 | MA6 | C5-C4 | 2.71 | 1.46 | 1.40 |
| 53 | DA | 745 | 1MG | C5-C4 | 2.71 | 1.46 | 1.40 |
| 1 | AA | 1516 | 2MG | C5-C4 | 2.74 | 1.46 | 1.40 |
| 53 | DA | 2457 | PSU | C4-N3 | 2.75 | 1.38 | 1.33 |
| 53 | DA | 2251 | OMG | C5-C4 | 2.76 | 1.46 | 1.40 |
| 22 | CA | 2457 | PSU | C4-N3 | 2.79 | 1.38 | 1.33 |
| 22 | CA | 955 | PSU | C4-N3 | 2.83 | 1.38 | 1.33 |
| 22 | CA | 2504 | PSU | C4-N3 | 2.88 | 1.38 | 1.33 |
| 53 | DA | 2069 | G7M | C6-C5 | 2.89 | 1.47 | 1.41 |
| 53 | DA | 1618 | 6MZ | C5-C4 | 2.91 | 1.47 | 1.40 |
| 1 | BA | 1518 | MA6 | C5-C4 | 2.92 | 1.47 | 1.40 |
| 1 | AA | 1207 | 2MG | C5-C4 | 2.92 | 1.47 | 1.40 |
| 22 | CA | 1915 | 3TD | C10-N3 | 2.92 | 1.53 | 1.47 |
| 1 | AA | 1518 | MA6 | C5-C4 | 2.94 | 1.47 | 1.40 |
| 1 | BA | 1207 | 2MG | C5-C4 | 2.94 | 1.47 | 1.40 |
| 53 | DA | 1835 | 2MG | C6-C5 | 2.96 | 1.47 | 1.41 |
| 1 | AA | 1516 | 2MG | C6-C5 | 2.97 | 1.47 | 1.41 |
| 53 | DA | 2503 | 2MA | C6-C5 | 2.97 | 1.46 | 1.41 |
| 22 | CA | 1835 | 2MG | C5-C4 | 3.02 | 1.47 | 1.40 |
| 53 | DA | 2445 | 2MG | C5-C4 | 3.02 | 1.47 | 1.40 |
| 53 | DA | 2580 | PSU | C4-N3 | 3.03 | 1.38 | 1.33 |
| 1 | AA | 516 | PSU | C4-N3 | 3.03 | 1.38 | 1.33 |
| 22 | CA | 2580 | PSU | C4-N3 | 3.08 | 1.38 | 1.33 |
| 53 | DA | 1917 | PSU | C4-N3 | 3.13 | 1.38 | 1.33 |
| 1 | BA | 966 | 2MG | C5-C4 | 3.13 | 1.47 | 1.40 |
| 1 | AA | 966 | 2MG | C5-C4 | 3.17 | 1.47 | 1.40 |
| 1 | AA | 1207 | 2MG | C6-C5 | 3.20 | 1.47 | 1.41 |
| 22 | CA | 745 | 1MG | C5-C4 | 3.21 | 1.47 | 1.40 |
| 22 | CA | 2445 | 2MG | C5-C4 | 3.23 | 1.47 | 1.40 |
| 22 | CA | 1618 | 6MZ | C5-C4 | 3.23 | 1.47 | 1.40 |
| 22 | CA | 2030 | 6MZ | C5-C4 | 3.24 | 1.47 | 1.40 |
| 1 | BA | 1516 | 2MG | C5-C4 | 3.28 | 1.47 | 1.40 |
| 53 | DA | 955 | PSU | C4-N3 | 3.30 | 1.39 | 1.33 |
| 22 | CA | 2251 | OMG | C5-C4 | 3.33 | 1.48 | 1.40 |
| 53 | DA | 2449 | H2U | C2-N1 | 3.33 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 22 | CA | 1917 | PSU | C4-N3 | 3.34 | 1.39 | 1.33 |
| 22 | CA | 1835 | 2MG | C6-C5 | 3.34 | 1.47 | 1.41 |
| 22 | CA | 1911 | PSU | C4-N3 | 3.36 | 1.39 | 1.33 |
| 53 | DA | 1911 | PSU | C4-N3 | 3.39 | 1.39 | 1.33 |
| 1 | BA | 527 | G7M | C6-C5 | 3.43 | 1.48 | 1.41 |
| 1 | AA | 966 | 2MG | C6-C5 | 3.52 | 1.48 | 1.41 |
| 53 | DA | 2251 | OMG | C6-C5 | 3.53 | 1.48 | 1.41 |
| 53 | DA | 2504 | PSU | C4-N3 | 3.57 | 1.39 | 1.33 |
| 22 | CA | 2503 | 2MA | C5-C4 | 3.60 | 1.48 | 1.40 |
| 53 | DA | 2445 | 2MG | C6-C5 | 3.63 | 1.48 | 1.41 |
| 1 | BA | 1516 | 2MG | C6-C5 | 3.64 | 1.48 | 1.41 |
| 22 | CA | 2251 | OMG | C6-C5 | 3.69 | 1.48 | 1.41 |
| 53 | DA | 2503 | 2MA | C6-N6 | 3.74 | 1.35 | 1.29 |
| 22 | CA | 2069 | G7M | C6-C5 | 3.75 | 1.48 | 1.41 |
| 1 | AA | 527 | G7M | C6-C5 | 3.80 | 1.48 | 1.41 |
| 1 | BA | 1207 | 2MG | C6-C5 | 3.86 | 1.49 | 1.41 |
| 1 | BA | 966 | 2MG | C6-C5 | 3.88 | 1.49 | 1.41 |
| 22 | CA | 2445 | 2MG | C6-C5 | 3.98 | 1.49 | 1.41 |
| 22 | CA | 2503 | 2MA | C6-N6 | 4.00 | 1.36 | 1.29 |
| 53 | DA | 745 | 1MG | C6-C5 | 4.06 | 1.48 | 1.41 |
| 22 | CA | 2503 | 2MA | C6-C5 | 4.09 | 1.48 | 1.41 |
| 53 | DA | 1962 | 5MC | C5-C4 | 4.18 | 1.47 | 1.41 |
| 1 | AA | 967 | 5MC | C5-C4 | 4.33 | 1.48 | 1.41 |
| 22 | CA | 745 | 1MG | C6-C5 | 4.34 | 1.49 | 1.41 |
| 22 | CA | 1962 | 5MC | C5-C4 | 4.81 | 1.48 | 1.41 |
| 1 | BA | 967 | 5MC | C5-C4 | 4.88 | 1.48 | 1.41 |
| 1 | AA | 1407 | 5MC | C5-C4 | 5.26 | 1.49 | 1.41 |
| 1 | BA | 1407 | 5MC | C5-C4 | 5.30 | 1.49 | 1.41 |

All (290) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 53 | DA | 2580 | PSU | N1-C2-N3 | -16.98 | 117.50 | 128.33 |
| 53 | DA | 2457 | PSU | N1-C2-N3 | -16.05 | 118.09 | 128.33 |
| 53 | DA | 2604 | PSU | N1-C2-N3 | -15.71 | 118.31 | 128.33 |
| 53 | DA | 955 | PSU | N1-C2-N3 | -14.73 | 118.94 | 128.33 |
| 53 | DA | 2504 | PSU | N1-C2-N3 | -14.45 | 119.11 | 128.33 |
| 53 | DA | 2605 | PSU | N1-C2-N3 | -13.78 | 119.54 | 128.33 |
| 22 | CA | 1917 | PSU | N1-C2-N3 | -13.66 | 119.62 | 128.33 |
| 22 | CA | 955 | PSU | N1-C2-N3 | -13.49 | 119.73 | 128.33 |
| 1 | BA | 516 | PSU | N1-C2-N3 | -13.47 | 119.74 | 128.33 |
| 53 | DA | 1911 | PSU | N1-C2-N3 | -13.18 | 119.92 | 128.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 22 | CA | 1911 | PSU | N1-C2-N3 | -13.17 | 119.93 | 128.33 |
| 1 | AA | 516 | PSU | N1-C2-N3 | -13.08 | 119.99 | 128.33 |
| 53 | DA | 1917 | PSU | N1-C2-N3 | -13.05 | 120.00 | 128.33 |
| 22 | CA | 2504 | PSU | N1-C2-N3 | -12.90 | 120.10 | 128.33 |
| 22 | CA | 2605 | PSU | N1-C2-N3 | -12.90 | 120.11 | 128.33 |
| 22 | CA | 2580 | PSU | N1-C2-N3 | -12.88 | 120.12 | 128.33 |
| 22 | CA | 2457 | PSU | N1-C2-N3 | -12.42 | 120.41 | 128.33 |
| 22 | CA | 746 | PSU | N1-C2-N3 | -11.46 | 121.02 | 128.33 |
| 53 | DA | 746 | PSU | N1-C2-N3 | -10.31 | 121.75 | 128.33 |
| 53 | DA | 2030 | 6MZ | N3-C2-N1 | -8.30 | 122.54 | 128.89 |
| 1 | BA | 1519 | MA6 | N3-C2-N1 | -8.25 | 122.58 | 128.89 |
| 1 | BA | 1518 | MA6 | N3-C2-N1 | -7.65 | 123.04 | 128.89 |
| 1 | AA | 1519 | MA6 | N3-C2-N1 | -7.58 | 123.09 | 128.89 |
| 22 | CA | 1618 | 6MZ | N3-C2-N1 | -7.35 | 123.26 | 128.89 |
| 22 | CA | 2030 | 6MZ | N3-C2-N1 | -7.25 | 123.34 | 128.89 |
| 53 | DA | 1939 | 5MU | C5-C4-N3 | -6.35 | 118.07 | 125.14 |
| 1 | AA | 1402 | 4OC | CM4-N4-C4 | -6.24 | 117.57 | 122.98 |
| 53 | DA | 1618 | 6MZ | N3-C2-N1 | -6.24 | 124.12 | 128.89 |
| 1 | AA | 1518 | MA6 | N3-C2-N1 | -6.19 | 124.15 | 128.89 |
| 22 | CA | 2504 | PSU | C5-C1'-C2' | -6.09 | 104.71 | 115.52 |
| 53 | DA | 2449 | H2U | C4-N3-C2 | -5.96 | 120.87 | 125.79 |
| 22 | CA | 1939 | 5MU | C5-C4-N3 | -5.54 | 118.97 | 125.14 |
| 53 | DA | 747 | 5MU | C5-C4-N3 | -5.46 | 119.06 | 125.14 |
| 53 | DA | 2445 | 2MG | C5-C6-N1 | -5.41 | 116.19 | 123.59 |
| 22 | CA | 2069 | G7M | C5-C6-N1 | -5.21 | 116.47 | 123.59 |
| 22 | CA | 747 | 5MU | C5-C4-N3 | -5.15 | 119.41 | 125.14 |
| 53 | DA | 2449 | H2U | C5-C6-N1 | -5.02 | 105.26 | 110.70 |
| 53 | DA | 2069 | G7M | C5-C6-N1 | -4.96 | 116.81 | 123.59 |
| 1 | BA | 527 | G7M | C5-C6-N1 | -4.88 | 116.92 | 123.59 |
| 1 | BA | 1516 | 2MG | CM2-N2-C2 | -4.78 | 117.68 | 123.07 |
| 1 | AA | 527 | G7M | C5-C6-N1 | -4.69 | 117.18 | 123.59 |
| 53 | DA | 2449 | H2U | C6-N1-C2 | -4.56 | 115.34 | 122.23 |
| 1 | AA | 966 | 2MG | C5-C6-N1 | -4.54 | 117.39 | 123.59 |
| 22 | CA | 2445 | 2MG | C5-C6-N1 | -4.52 | 117.41 | 123.59 |
| 53 | DA | 2504 | PSU | C5-C1'-C2' | -4.34 | 107.81 | 115.52 |
| 1 | AA | 1207 | 2MG | C5-C6-N1 | -4.22 | 117.82 | 123.59 |
| 53 | DA | 2251 | OMG | C5-C6-N1 | -4.14 | 117.93 | 123.59 |
| 53 | DA | 2445 | 2MG | C4-C5-N7 | -4.13 | 105.68 | 109.48 |
| 22 | CA | 1915 | 3TD | C5-C1'-C2' | -4.09 | 108.25 | 115.52 |
| 22 | CA | 1835 | 2MG | C5-C6-N1 | -4.05 | 118.05 | 123.59 |
| 1 | AA | 1516 | 2MG | C2'-C1'-N9 | -4.05 | 108.11 | 114.29 |
| 1 | AA | 966 | 2MG | CM2-N2-C2 | -4.01 | 118.54 | 123.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | CA | 1618 | 6MZ | C9-N6-C6 | -3.97 | 119.54 | 122.89 |
| 22 | CA | 1618 | 6MZ | C4-C5-N7 | -3.94 | 105.86 | 109.48 |
| 22 | CA | 2251 | OMG | C5-C6-N1 | -3.92 | 118.23 | 123.59 |
| 1 | BA | 1207 | 2MG | C6-C5-C4 | -3.89 | 116.24 | 120.90 |
| 1 | AA | 1207 | 2MG | CM2-N2-C2 | -3.88 | 118.69 | 123.07 |
| 1 | BA | 966 | 2MG | C5-C6-N1 | -3.88 | 118.28 | 123.59 |
| 22 | CA | 1915 | 3TD | C5-C6-N1 | -3.85 | 118.95 | 124.39 |
| 1 | BA | 1207 | 2MG | C5-C6-N1 | -3.84 | 118.34 | 123.59 |
| 53 | DA | 746 | PSU | C5-C1'-C2' | -3.82 | 108.73 | 115.52 |
| 53 | DA | 1835 | 2MG | CM2-N2-C2 | -3.82 | 118.76 | 123.07 |
| 22 | CA | 2030 | 6MZ | C9-N6-C6 | -3.82 | 119.66 | 122.89 |
| 1 | BA | 1516 | 2MG | C5-C6-N1 | -3.80 | 118.39 | 123.59 |
| 22 | CA | 2030 | 6MZ | C4-C5-N7 | -3.79 | 106.00 | 109.48 |
| 53 | DA | 745 | 1MG | C6-C5-C4 | -3.75 | 117.25 | 119.93 |
| 1 | AA | 1519 | MA6 | C4-C5-N7 | -3.67 | 106.10 | 109.48 |
| 1 | AA | 527 | G7M | C1'-N9-C4 | -3.67 | 121.41 | 126.94 |
| 53 | DA | 1835 | 2MG | C6-C5-C4 | -3.62 | 116.57 | 120.90 |
| 53 | DA | 2030 | 6MZ | C1'-N9-C4 | -3.60 | 121.51 | 126.94 |
| 22 | CA | 2445 | 2MG | C4-C5-N7 | -3.58 | 106.19 | 109.48 |
| 53 | DA | 745 | 1MG | C4-C5-N7 | -3.56 | 106.21 | 109.48 |
| 53 | DA | 1915 | 3TD | C5-C6-N1 | -3.55 | 119.37 | 124.39 |
| 53 | DA | 1618 | 6MZ | C4-C5-N7 | -3.51 | 106.25 | 109.48 |
| 22 | CA | 2605 | PSU | C5-C6-N1 | -3.51 | 119.44 | 124.39 |
| 1 | AA | 1516 | 2MG | C5-C6-N1 | -3.49 | 118.81 | 123.59 |
| 1 | BA | 1207 | 2MG | C4-C5-N7 | -3.47 | 106.29 | 109.48 |
| 53 | DA | 1915 | 3TD | C5-C1'-C2' | -3.45 | 109.39 | 115.52 |
| 1 | BA | 966 | 2MG | C4-C5-N7 | -3.45 | 106.31 | 109.48 |
| 22 | CA | 2251 | OMG | C6-C5-C4 | -3.42 | 116.81 | 120.90 |
| 1 | AA | 527 | G7M | C2'-C1'-N9 | -3.42 | 109.07 | 114.29 |
| 53 | DA | 2069 | G7M | N3-C2-N1 | -3.34 | 122.35 | 127.44 |
| 53 | DA | 2445 | 2MG | C6-C5-C4 | -3.33 | 116.91 | 120.90 |
| 22 | CA | 2445 | 2MG | CM2-N2-C2 | -3.33 | 119.31 | 123.07 |
| 53 | DA | 1618 | 6MZ | C9-N6-C6 | -3.29 | 120.11 | 122.89 |
| 1 | BA | 1516 | 2MG | C4-C5-N7 | -3.27 | 106.47 | 109.48 |
| 1 | BA | 1518 | MA6 | C4-C5-N7 | -3.23 | 106.51 | 109.48 |
| 22 | CA | 746 | PSU | C5-C6-N1 | -3.22 | 119.85 | 124.39 |
| 22 | CA | 2457 | PSU | C5-C6-N1 | -3.22 | 119.85 | 124.39 |
| 1 | BA | 1519 | MA6 | C2'-C1'-N9 | -3.21 | 109.39 | 114.29 |
| 22 | CA | 2251 | OMG | N3-C2-N1 | -3.19 | 122.58 | 127.44 |
| 1 | AA | 1207 | 2MG | C6-C5-C4 | -3.17 | 117.10 | 120.90 |
| 22 | CA | 1835 | 2MG | C6-C5-C4 | -3.17 | 117.11 | 120.90 |
| 53 | DA | 2604 | PSU | C5-C1'-C2' | -3.17 | 109.89 | 115.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22 | CA | 2605 | PSU | C5-C1'-C2' | -3.17 | 109.90 | 115.52 |
| 22 | CA | 2030 | 6MZ | C1'-N9-C4 | -3.16 | 122.18 | 126.94 |
| 53 | DA | 2251 | OMG | C6-C5-C4 | -3.15 | 117.14 | 120.90 |
| 1 | AA | 1516 | 2MG | C6-C5-C4 | -3.14 | 117.14 | 120.90 |
| 53 | DA | 1835 | 2MG | C4-C5-N7 | -3.14 | 106.59 | 109.48 |
| 22 | CA | 745 | 1MG | C4-C5-N7 | -3.13 | 106.60 | 109.48 |
| 22 | CA | 2445 | 2MG | C6-C5-C4 | -3.10 | 117.19 | 120.90 |
| 1 | BA | 1207 | 2MG | C1'-N9-C4 | -3.09 | 122.28 | 126.94 |
| 53 | DA | 2030 | 6MZ | C4-C5-N7 | -3.09 | 106.64 | 109.48 |
| 53 | DA | 2251 | OMG | C4-C5-N7 | -3.09 | 106.64 | 109.48 |
| 22 | CA | 2580 | PSU | C5-C6-N1 | -3.06 | 120.07 | 124.39 |
| 1 | AA | 1516 | 2MG | CM2-N2-C2 | -3.06 | 119.61 | 123.07 |
| 1 | BA | 966 | 2MG | C6-C5-C4 | -3.05 | 117.25 | 120.90 |
| 53 | DA | 1835 | 2MG | C5-C6-N1 | -3.03 | 119.45 | 123.59 |
| 22 | CA | 746 | PSU | C5-C1'-C2' | -3.02 | 110.15 | 115.52 |
| 1 | AA | 1519 | MA6 | C2'-C1'-N9 | -3.02 | 109.68 | 114.29 |
| 53 | DA | 2457 | PSU | C5-C6-N1 | -2.99 | 120.17 | 124.39 |
| 1 | AA | 966 | 2MG | C4-C5-N7 | -2.97 | 106.74 | 109.48 |
| 1 | AA | 1519 | MA6 | C1'-N9-C4 | -2.96 | 122.47 | 126.94 |
| 1 | BA | 527 | G7M | C2'-C1'-N9 | -2.96 | 109.77 | 114.29 |
| 1 | BA | 516 | PSU | C5-C6-N1 | -2.96 | 120.22 | 124.39 |
| 1 | BA | 1519 | MA6 | C4-C5-N7 | -2.96 | 106.76 | 109.48 |
| 22 | CA | 955 | PSU | C5-C6-N1 | -2.92 | 120.27 | 124.39 |
| 53 | DA | 1917 | PSU | C5-C6-N1 | -2.90 | 120.30 | 124.39 |
| 22 | CA | 2503 | 2MA | C4-C5-N7 | -2.89 | 106.82 | 109.48 |
| 1 | AA | 527 | G7M | N3-C2-N1 | -2.87 | 123.07 | 127.44 |
| 53 | DA | 2503 | 2MA | C1'-N9-C4 | -2.85 | 122.64 | 126.94 |
| 53 | DA | 1911 | PSU | C5-C6-N1 | -2.84 | 120.38 | 124.39 |
| 1 | BA | 1402 | 4OC | CM4-N4-C4 | -2.84 | 120.52 | 122.98 |
| 22 | CA | 2504 | PSU | C5-C6-N1 | -2.81 | 120.42 | 124.39 |
| 1 | AA | 1207 | 2MG | C4-C5-N7 | -2.80 | 106.90 | 109.48 |
| 53 | DA | 1917 | PSU | C5-C1'-C2' | -2.80 | 110.56 | 115.52 |
| 1 | AA | 966 | 2MG | C6-C5-C4 | -2.78 | 117.57 | 120.90 |
| 1 | BA | 966 | 2MG | CM2-N2-C2 | -2.77 | 119.95 | 123.07 |
| 53 | DA | 2503 | 2MA | C4-C5-N7 | -2.76 | 106.94 | 109.48 |
| 53 | DA | 746 | PSU | C5-C6-N1 | -2.75 | 120.51 | 124.39 |
| 53 | DA | 2605 | PSU | C5-C6-N1 | -2.73 | 120.54 | 124.39 |
| 22 | CA | 1911 | PSU | C5-C6-N1 | -2.71 | 120.56 | 124.39 |
| 1 | BA | 1207 | 2MG | N3-C2-N1 | -2.68 | 122.10 | 126.22 |
| 1 | AA | 1518 | MA6 | C4-C5-N7 | -2.68 | 107.01 | 109.48 |
| 22 | CA | 2069 | G7M | N3-C2-N1 | -2.68 | 123.37 | 127.44 |
| 53 | DA | 1835 | 2MG | N3-C2-N1 | -2.67 | 122.11 | 126.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 22 | CA | 1835 | 2MG | C4-C5-N7 | -2.66 | 107.03 | 109.48 |
| 1 | AA | 1516 | 2MG | C4-C5-N7 | -2.64 | 107.05 | 109.48 |
| 22 | CA | 1835 | 2MG | N3-C2-N1 | -2.64 | 122.16 | 126.22 |
| 53 | DA | 2069 | G7M | C6-C5-C4 | -2.63 | 117.75 | 120.90 |
| 53 | DA | 2449 | H2U | O2-C2-N1 | -2.63 | 119.87 | 123.30 |
| 53 | DA | 2030 | 6MZ | C9-N6-C6 | -2.62 | 120.68 | 122.89 |
| 1 | BA | 1516 | 2MG | C6-C5-C4 | -2.56 | 117.83 | 120.90 |
| 22 | CA | 2503 | 2MA | C1'-N9-C4 | -2.56 | 123.09 | 126.94 |
| 1 | AA | 1207 | 2MG | N3-C2-N1 | -2.52 | 122.34 | 126.22 |
| 22 | CA | 2251 | OMG | C4-C5-N7 | -2.50 | 107.18 | 109.48 |
| 1 | AA | 967 | 5MC | C5-C4-N4 | -2.46 | 118.57 | 122.20 |
| 1 | AA | 516 | PSU | C5-C6-N1 | -2.45 | 120.93 | 124.39 |
| 1 | BA | 1519 | MA6 | C1'-N9-C4 | -2.43 | 123.27 | 126.94 |
| 1 | BA | 527 | G7M | N3-C2-N1 | -2.40 | 123.78 | 127.44 |
| 22 | CA | 745 | 1MG | C6-C5-C4 | -2.37 | 118.23 | 119.93 |
| 53 | DA | 2251 | OMG | N3-C2-N1 | -2.36 | 123.85 | 127.44 |
| 1 | AA | 527 | G7M | C6-C5-C4 | -2.33 | 118.11 | 120.90 |
| 1 | BA | 1207 | 2MG | CM2-N2-C2 | -2.33 | 120.44 | 123.07 |
| 54 | DD | 150[A] | MEQ | OE1-CD-CG | -2.33 | 117.97 | 121.98 |
| 22 | CA | 1917 | PSU | C5-C6-N1 | -2.32 | 121.11 | 124.39 |
| 1 | AA | 1207 | 2MG | C2'-C1'-N9 | -2.32 | 110.75 | 114.29 |
| 53 | DA | 2604 | PSU | C5-C6-N1 | -2.29 | 121.17 | 124.39 |
| 1 | BA | 1207 | 2MG | C2'-C1'-N9 | -2.26 | 110.84 | 114.29 |
| 22 | CA | 2251 | OMG | C1'-N9-C4 | -2.22 | 123.58 | 126.94 |
| 22 | CA | 1835 | 2MG | CM2-N2-C2 | -2.22 | 120.57 | 123.07 |
| 22 | CA | 2445 | 2MG | N3-C2-N1 | -2.21 | 122.81 | 126.22 |
| 1 | BA | 966 | 2MG | N3-C2-N1 | -2.20 | 122.84 | 126.22 |
| 22 | CA | 1618 | 6MZ | C1'-N9-C4 | -2.16 | 123.68 | 126.94 |
| 1 | BA | 1402 | 4OC | C5-C4-N3 | -2.10 | 119.48 | 123.24 |
| 53 | DA | 2251 | OMG | C1'-N9-C4 | -2.10 | 123.78 | 126.94 |
| 1 | AA | 966 | 2MG | N3-C2-N1 | -2.09 | 123.01 | 126.22 |
| 53 | DA | 2445 | 2MG | C1'-N9-C4 | -2.08 | 123.81 | 126.94 |
| 34 | DN | 81[B] | 4D4 | OB-CB-CA | -2.06 | 104.83 | 109.66 |
| 53 | DA | 2605 | PSU | C5-C1'-C2' | -2.06 | 111.86 | 115.52 |
| 53 | DA | 2445 | 2MG | N3-C2-N1 | -2.05 | 123.06 | 126.22 |
| 22 | CA | 2251 | OMG | CM2-O2'-C2' | -2.05 | 108.80 | 114.59 |
| 22 | CA | 2498 | OMC | N4-C4-N3 | 2.01 | 120.17 | 116.50 |
| 22 | CA | 1835 | 2MG | N2-C2-N3 | 2.02 | 119.28 | 116.94 |
| 22 | CA | 1917 | PSU | O4'-C1'-C2' | 2.02 | 106.79 | 104.73 |
| 53 | DA | 1962 | 5MC | N4-C4-N3 | 2.08 | 119.96 | 116.95 |
| 53 | DA | 1618 | 6MZ | N6-C6-N1 | 2.14 | 121.25 | 118.77 |
| 22 | CA | 955 | PSU | O4'-C1'-C2' | 2.16 | 106.93 | 104.73 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 53 | DA | 1911 | PSU | O4'-C1'-C2' | 2.22 | 107.00 | 104.73 |
| 53 | DA | 2457 | PSU | O4'-C1'-C2' | 2.24 | 107.01 | 104.73 |
| 12 | BL | 89 | D2T | CB-CA-N | 2.24 | 114.50 | 109.66 |
| 53 | DA | 2580 | PSU | C4-C5-C1' | 2.29 | 125.42 | 121.23 |
| 1 | BA | 1207 | 2MG | N2-C2-N1 | 2.31 | 119.62 | 116.94 |
| 1 | AA | 1207 | 2MG | N2-C2-N1 | 2.34 | 119.65 | 116.94 |
| 53 | DA | 2449 | H2U | C1'-N1-C2 | 2.35 | 121.53 | 118.27 |
| 22 | CA | 2605 | PSU | O4'-C1'-C2' | 2.38 | 107.16 | 104.73 |
| 1 | BA | 1407 | 5MC | N4-C4-N3 | 2.39 | 120.41 | 116.95 |
| 22 | CA | 1911 | PSU | O4'-C1'-C2' | 2.40 | 107.17 | 104.73 |
| 1 | AA | 516 | PSU | O4'-C1'-C2' | 2.43 | 107.21 | 104.73 |
| 53 | DA | 746 | PSU | C6-N1-C2 | 2.45 | 119.41 | 115.47 |
| 53 | DA | 1917 | PSU | O4'-C1'-C2' | 2.52 | 107.30 | 104.73 |
| 1 | AA | 1407 | 5MC | N4-C4-N3 | 2.53 | 120.61 | 116.95 |
| 1 | BA | 516 | PSU | O4'-C1'-C2' | 2.56 | 107.34 | 104.73 |
| 1 | BA | 967 | 5MC | N4-C4-N3 | 2.58 | 120.68 | 116.95 |
| 53 | DA | 1915 | 3TD | O4'-C1'-C2' | 2.65 | 107.43 | 104.73 |
| 53 | DA | 2498 | OMC | N4-C4-N3 | 2.70 | 121.42 | 116.50 |
| 22 | CA | 2457 | PSU | O4'-C1'-C2' | 2.78 | 107.56 | 104.73 |
| 22 | CA | 2504 | PSU | C6-N1-C2 | 2.83 | 120.02 | 115.47 |
| 53 | DA | 2445 | 2MG | N2-C2-N1 | 2.84 | 120.23 | 116.94 |
| 22 | CA | 746 | PSU | C6-N1-C2 | 2.88 | 120.10 | 115.47 |
| 53 | DA | 955 | PSU | C6-N1-C2 | 2.95 | 120.21 | 115.47 |
| 22 | CA | 2457 | PSU | C6-N1-C2 | 2.97 | 120.25 | 115.47 |
| 53 | DA | 1917 | PSU | C6-N1-C2 | 3.03 | 120.34 | 115.47 |
| 22 | CA | 1962 | 5MC | N4-C4-N3 | 3.04 | 121.35 | 116.95 |
| 1 | BA | 516 | PSU | C6-N1-C2 | 3.10 | 120.45 | 115.47 |
| 22 | CA | 2580 | PSU | C6-N1-C2 | 3.13 | 120.50 | 115.47 |
| 53 | DA | 2498 | OMC | C2-N3-C4 | 3.17 | 120.08 | 115.61 |
| 22 | CA | 1911 | PSU | C6-N1-C2 | 3.20 | 120.61 | 115.47 |
| 1 | AA | 516 | PSU | C6-N1-C2 | 3.23 | 120.66 | 115.47 |
| 53 | DA | 2580 | PSU | O4'-C1'-C2' | 3.27 | 108.07 | 104.73 |
| 22 | CA | 1917 | PSU | C6-N1-C2 | 3.30 | 120.78 | 115.47 |
| 22 | CA | 2498 | OMC | C2-N3-C4 | 3.33 | 120.32 | 115.61 |
| 22 | CA | 2605 | PSU | C6-N1-C2 | 3.35 | 120.85 | 115.47 |
| 53 | DA | 2604 | PSU | C6-N1-C2 | 3.38 | 120.90 | 115.47 |
| 53 | DA | 2504 | PSU | C6-N1-C2 | 3.39 | 120.91 | 115.47 |
| 1 | BA | 1519 | MA6 | N1-C6-N6 | 3.46 | 120.81 | 117.05 |
| 53 | DA | 2449 | H2U | C5-C4-N3 | 3.46 | 119.97 | 116.71 |
| 22 | CA | 1915 | 3TD | O4'-C1'-C2' | 3.47 | 108.27 | 104.73 |
| 1 | AA | 967 | 5MC | N4-C4-N3 | 3.49 | 122.01 | 116.95 |
| 53 | DA | 2605 | PSU | C6-N1-C2 | 3.49 | 121.09 | 115.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 53 | DA | 1911 | PSU | C6-N1-C2 | 3.58 | 121.22 | 115.47 |
| 22 | CA | 955 | PSU | C6-N1-C2 | 3.64 | 121.33 | 115.47 |
| 53 | DA | 2449 | H2U | N3-C2-N1 | 3.66 | 120.25 | 116.60 |
| 53 | DA | 1835 | 2MG | C6-N1-C2 | 3.80 | 120.84 | 115.31 |
| 53 | DA | 1915 | 3TD | C6-N1-C2 | 3.83 | 121.62 | 115.47 |
| 22 | CA | 2580 | PSU | O4'-C1'-C2' | 3.87 | 108.68 | 104.73 |
| 53 | DA | 1835 | 2MG | N2-C2-N1 | 3.89 | 121.46 | 116.94 |
| 53 | DA | 2457 | PSU | C6-N1-C2 | 4.00 | 121.90 | 115.47 |
| 53 | DA | 2580 | PSU | C6-N1-C2 | 4.01 | 121.92 | 115.47 |
| 1 | AA | 1516 | 2MG | C6-N1-C2 | 4.05 | 121.20 | 115.31 |
| 53 | DA | 2251 | OMG | C6-N1-C2 | 4.08 | 121.61 | 115.94 |
| 53 | DA | 2445 | 2MG | C2-N3-C4 | 4.17 | 120.11 | 115.09 |
| 1 | AA | 1516 | 2MG | C2-N3-C4 | 4.18 | 120.12 | 115.09 |
| 53 | DA | 1911 | PSU | C4-N3-C2 | 4.26 | 118.93 | 115.25 |
| 1 | AA | 527 | G7M | C6-N1-C2 | 4.26 | 121.85 | 115.94 |
| 22 | CA | 1915 | 3TD | C6-N1-C2 | 4.27 | 122.34 | 115.47 |
| 1 | BA | 1516 | 2MG | C6-N1-C2 | 4.29 | 121.55 | 115.31 |
| 1 | AA | 966 | 2MG | C2-N3-C4 | 4.34 | 120.31 | 115.09 |
| 1 | BA | 527 | G7M | C6-N1-C2 | 4.35 | 121.98 | 115.94 |
| 1 | AA | 1207 | 2MG | C2-N3-C4 | 4.53 | 120.54 | 115.09 |
| 1 | AA | 1518 | MA6 | C2-N1-C6 | 4.68 | 121.39 | 111.43 |
| 22 | CA | 2069 | G7M | C6-N1-C2 | 4.68 | 122.44 | 115.94 |
| 1 | AA | 516 | PSU | C4-N3-C2 | 4.69 | 119.30 | 115.25 |
| 22 | CA | 2445 | 2MG | C2-N3-C4 | 4.72 | 120.77 | 115.09 |
| 1 | BA | 966 | 2MG | C6-N1-C2 | 4.72 | 122.17 | 115.31 |
| 22 | CA | 955 | PSU | C4-N3-C2 | 4.76 | 119.36 | 115.25 |
| 53 | DA | 2605 | PSU | C4-N3-C2 | 4.82 | 119.41 | 115.25 |
| 22 | CA | 2251 | OMG | C6-N1-C2 | 4.83 | 122.64 | 115.94 |
| 1 | AA | 966 | 2MG | C6-N1-C2 | 4.86 | 122.39 | 115.31 |
| 1 | BA | 1516 | 2MG | C2-N3-C4 | 4.90 | 120.98 | 115.09 |
| 53 | DA | 746 | PSU | C4-N3-C2 | 4.92 | 119.50 | 115.25 |
| 1 | AA | 1519 | MA6 | C2-N1-C6 | 4.93 | 121.92 | 111.43 |
| 22 | CA | 1835 | 2MG | C2-N3-C4 | 4.93 | 121.03 | 115.09 |
| 1 | BA | 1518 | MA6 | C2-N1-C6 | 4.95 | 121.97 | 111.43 |
| 22 | CA | 2605 | PSU | C4-N3-C2 | 4.95 | 119.53 | 115.25 |
| 1 | BA | 1207 | 2MG | C2-N3-C4 | 4.99 | 121.10 | 115.09 |
| 1 | BA | 1207 | 2MG | C6-N1-C2 | 5.04 | 122.64 | 115.31 |
| 22 | CA | 2504 | PSU | C4-N3-C2 | 5.07 | 119.63 | 115.25 |
| 1 | AA | 1207 | 2MG | C6-N1-C2 | 5.08 | 122.69 | 115.31 |
| 53 | DA | 2069 | G7M | C6-N1-C2 | 5.09 | 123.01 | 115.94 |
| 22 | CA | 2580 | PSU | C4-N3-C2 | 5.12 | 119.67 | 115.25 |
| 22 | CA | 2445 | 2MG | C6-N1-C2 | 5.13 | 122.77 | 115.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 22 | CA | 1911 | PSU | C4-N3-C2 | 5.14 | 119.69 | 115.25 |
| 22 | CA | 747 | 5MU | C4-N3-C2 | 5.15 | 119.69 | 115.25 |
| 1 | BA | 1519 | MA6 | C2-N1-C6 | 5.17 | 122.44 | 111.43 |
| 22 | CA | 1835 | 2MG | C6-N1-C2 | 5.19 | 122.86 | 115.31 |
| 1 | BA | 966 | 2MG | C2-N3-C4 | 5.20 | 121.36 | 115.09 |
| 22 | CA | 746 | PSU | C4-N3-C2 | 5.21 | 119.75 | 115.25 |
| 22 | CA | 2457 | PSU | C4-N3-C2 | 5.23 | 119.77 | 115.25 |
| 53 | DA | 2604 | PSU | C4-N3-C2 | 5.41 | 119.92 | 115.25 |
| 53 | DA | 747 | 5MU | C4-N3-C2 | 5.51 | 120.01 | 115.25 |
| 53 | DA | 1917 | PSU | C4-N3-C2 | 5.73 | 120.20 | 115.25 |
| 53 | DA | 2445 | 2MG | C6-N1-C2 | 5.78 | 123.72 | 115.31 |
| 22 | CA | 1917 | PSU | C4-N3-C2 | 5.79 | 120.25 | 115.25 |
| 1 | BA | 516 | PSU | C4-N3-C2 | 5.84 | 120.29 | 115.25 |
| 53 | DA | 2457 | PSU | C4-N3-C2 | 6.01 | 120.44 | 115.25 |
| 53 | DA | 1835 | 2MG | C2-N3-C4 | 6.01 | 122.32 | 115.09 |
| 53 | DA | 2504 | PSU | C4-N3-C2 | 6.17 | 120.58 | 115.25 |
| 53 | DA | 2552 | OMU | C4-N3-C2 | 6.30 | 120.38 | 114.14 |
| 22 | CA | 2552 | OMU | C4-N3-C2 | 6.51 | 120.59 | 114.14 |
| 53 | DA | 2580 | PSU | C4-N3-C2 | 6.55 | 120.91 | 115.25 |
| 22 | CA | 1939 | 5MU | C4-N3-C2 | 6.60 | 120.95 | 115.25 |
| 53 | DA | 955 | PSU | C4-N3-C2 | 7.12 | 121.40 | 115.25 |
| 53 | DA | 1939 | 5MU | C4-N3-C2 | 7.18 | 121.45 | 115.25 |
| 53 | DA | 1618 | 6MZ | C2-N1-C6 | 7.97 | 122.22 | 116.48 |
| 22 | CA | 2503 | 2MA | C2-N3-C4 | 8.03 | 119.69 | 115.34 |
| 22 | CA | 1618 | 6MZ | C2-N1-C6 | 8.10 | 122.31 | 116.48 |
| 53 | DA | 2503 | 2MA | C2-N3-C4 | 8.39 | 119.89 | 115.34 |
| 22 | CA | 2030 | 6MZ | C2-N1-C6 | 9.33 | 123.20 | 116.48 |
| 53 | DA | 2030 | 6MZ | C2-N1-C6 | 9.63 | 123.41 | 116.48 |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|--------|------|--------------|
| 54 | DD | 150[B] | MEQ | CG-CD-NE2-CE |

There are no ring outliers.

31 monomers are involved in 47 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 1 | AA | 1402 | 4OC | 1 | 0 |
| 1 | AA | 1518 | MA6 | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 1 | AA | 1519 | MA6 | 3 | 0 |
| 1 | AA | 527 | G7M | 2 | 0 |
| 1 | BA | 1402 | 4OC | 2 | 0 |
| 1 | BA | 1407 | 5MC | 2 | 0 |
| 1 | BA | 1498 | UR3 | 1 | 0 |
| 1 | BA | 1516 | 2MG | 1 | 0 |
| 1 | BA | 1518 | MA6 | 2 | 0 |
| 1 | BA | 1519 | MA6 | 4 | 0 |
| 1 | BA | 516 | PSU | 1 | 0 |
| 1 | BA | 966 | 2MG | 1 | 0 |
| 1 | BA | 967 | 5MC | 1 | 0 |
| 22 | CA | 1618 | 6MZ | 1 | 0 |
| 22 | CA | 1915 | 3TD | 6 | 0 |
| 22 | CA | 1939 | 5MU | 1 | 0 |
| 22 | CA | 1962 | 5MC | 1 | 0 |
| 22 | CA | 2030 | 6MZ | 2 | 0 |
| 22 | CA | 2069 | G7M | 1 | 0 |
| 22 | CA | 2251 | OMG | 1 | 0 |
| 22 | CA | 2445 | 2MG | 2 | 0 |
| 22 | CA | 2498 | OMC | 2 | 0 |
| 22 | CA | 2503 | 2MA | 4 | 0 |
| 22 | CA | 747 | 5MU | 1 | 0 |
| 34 | CN | 81 | 4D4 | 1 | 0 |
| 53 | DA | 2030 | 6MZ | 2 | 0 |
| 53 | DA | 2251 | OMG | 2 | 0 |
| 53 | DA | 2498 | OMC | 2 | 0 |
| 54 | DD | 150[A] | MEQ | 1 | 0 |
| 54 | DD | 150[B] | MEQ | 1 | 0 |
| 34 | DN | 81[A] | 4D4 | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 546 ligands modelled in this entry, 466 are monoatomic - leaving 80 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 57 | PG4 | AA | 1670 | - | 12,12,12 | 0.81 | 0 | 11,11,11 | 0.41 | 0 |
| 58 | MPD | AA | 1671 | - | 6,7,7 | 0.52 | 0 | 7,10,10 | 0.56 | 0 |
| 59 | PUT | AA | 1672 | - | 5,5,5 | 0.24 | 0 | 4,4,4 | 0.79 | 0 |
| 59 | PUT | AA | 1673 | - | 5,5,5 | 0.25 | 0 | 4,4,4 | 0.70 | 0 |
| 59 | PUT | AA | 1674 | - | 5,5,5 | 0.23 | 0 | 4,4,4 | 0.75 | 0 |
| 59 | PUT | AA | 1675 | - | 5,5,5 | 0.31 | 0 | 4,4,4 | 0.52 | 0 |
| 58 | MPD | AA | 1676 | - | 6,7,7 | 0.67 | 0 | 7,10,10 | 0.59 | 0 |
| 61 | PEG | AL | 201 | - | 6,6,6 | 0.95 | 0 | 5,5,5 | 0.47 | 0 |
| 57 | PG4 | BA | 1642 | - | 12,12,12 | 0.80 | 0 | 11,11,11 | 0.44 | 0 |
| 66 | EDO | D0 | 101 | - | 3,3,3 | 0.39 | 0 | 2,2,2 | 0.51 | 0 |
| 66 | EDO | D1 | 101 | - | 3,3,3 | 0.29 | 0 | 2,2,2 | 0.50 | 0 |
| 64 | PGE | D1 | 102 | - | 9,9,9 | 1.04 | 0 | 8,8,8 | 0.31 | 0 |
| 64 | PGE | D3 | 101 | - | 9,9,9 | 0.91 | 0 | 8,8,8 | 0.38 | 0 |
| 61 | PEG | D3 | 102 | - | 6,6,6 | 0.98 | 0 | 5,5,5 | 0.40 | 0 |
| 62 | SPD | DA | 3183 | - | 9,9,9 | 0.43 | 0 | 8,8,8 | 0.82 | 0 |
| 59 | PUT | DA | 3184 | - | 5,5,5 | 0.31 | 0 | 4,4,4 | 0.48 | 0 |
| 63 | 1PE | DA | 3185 | - | 15,15,15 | 0.55 | 0 | 14,14,14 | 0.49 | 0 |
| 64 | PGE | DA | 3186 | - | 9,9,9 | 0.92 | 0 | 8,8,8 | 0.30 | 0 |
| 62 | SPD | DA | 3187 | - | 9,9,9 | 0.42 | 0 | 8,8,8 | 0.91 | 0 |
| 59 | PUT | DA | 3188 | - | 5,5,5 | 0.20 | 0 | 4,4,4 | 0.33 | 0 |
| 59 | PUT | DA | 3189 | - | 5,5,5 | 0.34 | 0 | 4,4,4 | 0.54 | 0 |
| 58 | MPD | DA | 3190 | - | 6,7,7 | 0.52 | 0 | 7,10,10 | 0.69 | 0 |
| 65 | ACY | DA | 3191 | - | 1,3,3 | 2.32 | 1 (100%) | 0,3,3 | 0.00 | - |
| 58 | MPD | DA | 3192 | - | 6,7,7 | 0.37 | 0 | 7,10,10 | 1.35 | 1 (14%) |
| 57 | PG4 | DA | 3193 | - | 12,12,12 | 0.79 | 0 | 11,11,11 | 0.60 | 0 |
| 66 | EDO | DA | 3194 | - | 3,3,3 | 0.34 | 0 | 2,2,2 | 0.53 | 0 |
| 59 | PUT | DA | 3195 | - | 5,5,5 | 0.30 | 0 | 4,4,4 | 0.46 | 0 |
| 65 | ACY | DA | 3196 | - | 1,3,3 | 3.25 | 1 (100%) | 0,3,3 | 0.00 | - |
| 66 | EDO | DA | 3197 | - | 3,3,3 | 0.31 | 0 | 2,2,2 | 0.63 | 0 |
| 66 | EDO | DA | 3198 | - | 3,3,3 | 0.37 | 0 | 2,2,2 | 0.45 | 0 |
| 61 | PEG | DA | 3199 | - | 6,6,6 | 0.91 | 0 | 5,5,5 | 0.60 | 0 |
| 61 | PEG | DA | 3200 | - | 6,6,6 | 1.05 | 0 | 5,5,5 | 0.54 | 0 |
| 61 | PEG | DA | 3201 | - | 6,6,6 | 1.02 | 0 | 5,5,5 | 0.51 | 0 |
| 65 | ACY | DA | 3202 | - | 1,3,3 | 2.23 | 1 (100%) | 0,3,3 | 0.00 | - |
| 63 | 1PE | DA | 3203 | - | 15,15,15 | 0.65 | 0 | 14,14,14 | 0.33 | 0 |
| 64 | PGE | DA | 3204 | - | 9,9,9 | 0.96 | 0 | 8,8,8 | 0.54 | 0 |
| 58 | MPD | DA | 3205 | - | 6,7,7 | 0.66 | 0 | 7,10,10 | 1.19 | 1 (14%) |
| 59 | PUT | DA | 3206 | - | 5,5,5 | 0.31 | 0 | 4,4,4 | 0.73 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 62 | SPD | DA | 3207 | - | 9,9,9 | 0.51 | 0 | 8,8,8 | 0.70 | 0 |
| 58 | MPD | DA | 3208 | - | 6,7,7 | 0.52 | 0 | 7,10,10 | 0.41 | 0 |
| 66 | EDO | DA | 3209 | - | 3,3,3 | 0.40 | 0 | 2,2,2 | 0.38 | 0 |
| 66 | EDO | DA | 3210 | - | 3,3,3 | 0.35 | 0 | 2,2,2 | 0.56 | 0 |
| 58 | MPD | DA | 3211 | - | 6,7,7 | 0.49 | 0 | 7,10,10 | 0.92 | 1 (14%) |
| 67 | GUN | DA | 3212 | - | 9,12,12 | 2.08 | 2 (22%) | 7,17,17 | 3.03 | 5 (71%) |
| 59 | PUT | DA | 3213 | - | 5,5,5 | 0.29 | 0 | 4,4,4 | 0.35 | 0 |
| 59 | PUT | DA | 3214 | - | 5,5,5 | 0.26 | 0 | 4,4,4 | 0.62 | 0 |
| 64 | PGE | DA | 3215 | - | 9,9,9 | 0.92 | 0 | 8,8,8 | 0.30 | 0 |
| 66 | EDO | DA | 3216 | - | 3,3,3 | 0.41 | 0 | 2,2,2 | 0.43 | 0 |
| 57 | PG4 | DA | 3217 | - | 12,12,12 | 0.74 | 0 | 11,11,11 | 0.55 | 0 |
| 64 | PGE | DA | 3218 | - | 9,9,9 | 0.83 | 0 | 8,8,8 | 0.38 | 0 |
| 61 | PEG | DA | 3219 | - | 6,6,6 | 1.01 | 0 | 5,5,5 | 0.45 | 0 |
| 59 | PUT | DA | 3220 | - | 5,5,5 | 0.21 | 0 | 4,4,4 | 0.67 | 0 |
| 68 | TRS | DA | 3221 | - | 7,7,7 | 0.88 | 0 | 9,9,9 | 1.01 | 1 (11%) |
| 59 | PUT | DA | 3222 | - | 5,5,5 | 0.24 | 0 | 4,4,4 | 0.65 | 0 |
| 59 | PUT | DA | 3223 | - | 5,5,5 | 0.35 | 0 | 4,4,4 | 0.56 | 0 |
| 59 | PUT | DA | 3224 | - | 5,5,5 | 0.21 | 0 | 4,4,4 | 0.97 | 0 |
| 62 | SPD | DA | 3225 | - | 9,9,9 | 0.56 | 0 | 8,8,8 | 1.04 | 1 (12%) |
| 64 | PGE | DA | 3226 | - | 9,9,9 | 0.95 | 0 | 8,8,8 | 0.27 | 0 |
| 61 | PEG | DA | 3227 | - | 6,6,6 | 0.95 | 0 | 5,5,5 | 0.43 | 0 |
| 61 | PEG | DA | 3228 | - | 6,6,6 | 1.03 | 0 | 5,5,5 | 0.17 | 0 |
| 66 | EDO | DB | 210 | - | 3,3,3 | 0.32 | 0 | 2,2,2 | 0.83 | 0 |
| 66 | EDO | DB | 211 | - | 3,3,3 | 0.40 | 0 | 2,2,2 | 0.57 | 0 |
| 66 | EDO | DB | 212 | - | 3,3,3 | 0.36 | 0 | 2,2,2 | 0.53 | 0 |
| 58 | MPD | DE | 301 | - | 6,7,7 | 0.61 | 0 | 7,10,10 | 0.47 | 0 |
| 58 | MPD | DE | 302 | - | 6,7,7 | 0.51 | 0 | 7,10,10 | 0.64 | 0 |
| 58 | MPD | DK | 201 | - | 6,7,7 | 0.53 | 0 | 7,10,10 | 0.64 | 0 |
| 61 | PEG | DL | 201 | - | 6,6,6 | 0.85 | 0 | 5,5,5 | 0.56 | 0 |
| 59 | PUT | DM | 201 | - | 5,5,5 | 0.25 | 0 | 4,4,4 | 0.86 | 0 |
| 58 | MPD | DN | 201 | - | 6,7,7 | 0.51 | 0 | 7,10,10 | 0.67 | 0 |
| 61 | PEG | DP | 201 | - | 6,6,6 | 0.97 | 0 | 5,5,5 | 0.42 | 0 |
| 61 | PEG | DQ | 201 | - | 6,6,6 | 0.99 | 0 | 5,5,5 | 0.49 | 0 |
| 57 | PG4 | DQ | 202 | - | 12,12,12 | 0.66 | 0 | 11,11,11 | 0.57 | 0 |
| 57 | PG4 | DR | 202 | - | 12,12,12 | 0.85 | 0 | 11,11,11 | 0.40 | 0 |
| 66 | EDO | DR | 203 | - | 3,3,3 | 0.33 | 0 | 2,2,2 | 0.46 | 0 |
| 64 | PGE | DS | 201 | - | 9,9,9 | 0.95 | 0 | 8,8,8 | 0.31 | 0 |
| 57 | PG4 | DS | 202 | - | 12,12,12 | 0.76 | 0 | 11,11,11 | 0.31 | 0 |
| 58 | MPD | DS | 203 | - | 6,7,7 | 0.88 | 0 | 7,10,10 | 0.64 | 0 |
| 58 | MPD | DT | 201 | - | 6,7,7 | 0.77 | 0 | 7,10,10 | 0.79 | 0 |
| 58 | MPD | DT | 202 | - | 6,7,7 | 0.51 | 0 | 7,10,10 | 0.56 | 0 |
| 64 | PGE | DU | 101 | - | 9,9,9 | 0.96 | 0 | 8,8,8 | 0.45 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 57 | PG4 | AA | 1670 | - | - | 0/10/10/10 | 0/0/0/0 |
| 58 | MPD | AA | 1671 | - | - | 0/5/5/5 | 0/0/0/0 |
| 59 | PUT | AA | 1672 | - | - | 0/3/3/3 | 0/0/0/0 |
| 59 | PUT | AA | 1673 | - | - | 0/3/3/3 | 0/0/0/0 |
| 59 | PUT | AA | 1674 | - | - | 0/3/3/3 | 0/0/0/0 |
| 59 | PUT | AA | 1675 | - | - | 0/3/3/3 | 0/0/0/0 |
| 58 | MPD | AA | 1676 | - | - | 0/5/5/5 | 0/0/0/0 |
| 61 | PEG | AL | 201 | - | - | 0/4/4/4 | 0/0/0/0 |
| 57 | PG4 | BA | 1642 | - | - | 0/10/10/10 | 0/0/0/0 |
| 66 | EDO | D0 | 101 | - | - | 0/1/1/1 | 0/0/0/0 |
| 66 | EDO | D1 | 101 | - | - | 0/1/1/1 | 0/0/0/0 |
| 64 | PGE | D1 | 102 | - | - | 0/7/7/7 | 0/0/0/0 |
| 64 | PGE | D3 | 101 | - | - | 0/7/7/7 | 0/0/0/0 |
| 61 | PEG | D3 | 102 | - | - | 0/4/4/4 | 0/0/0/0 |
| 62 | SPD | DA | 3183 | - | - | 0/7/7/7 | 0/0/0/0 |
| 59 | PUT | DA | 3184 | - | - | 0/3/3/3 | 0/0/0/0 |
| 63 | 1PE | DA | 3185 | - | - | 0/13/13/13 | 0/0/0/0 |
| 64 | PGE | DA | 3186 | - | - | 0/7/7/7 | 0/0/0/0 |
| 62 | SPD | DA | 3187 | - | - | 0/7/7/7 | 0/0/0/0 |
| 59 | PUT | DA | 3188 | - | - | 0/3/3/3 | 0/0/0/0 |
| 59 | PUT | DA | 3189 | - | - | 0/3/3/3 | 0/0/0/0 |
| 58 | MPD | DA | 3190 | - | - | 0/5/5/5 | 0/0/0/0 |
| 65 | ACY | DA | 3191 | - | - | 0/0/0/0 | 0/0/0/0 |
| 58 | MPD | DA | 3192 | - | - | 0/5/5/5 | 0/0/0/0 |
| 57 | PG4 | DA | 3193 | - | - | 0/10/10/10 | 0/0/0/0 |
| 66 | EDO | DA | 3194 | - | - | 0/1/1/1 | 0/0/0/0 |
| 59 | PUT | DA | 3195 | - | - | 0/3/3/3 | 0/0/0/0 |
| 65 | ACY | DA | 3196 | - | - | 0/0/0/0 | 0/0/0/0 |
| 66 | EDO | DA | 3197 | - | - | 0/1/1/1 | 0/0/0/0 |
| 66 | EDO | DA | 3198 | - | - | 0/1/1/1 | 0/0/0/0 |
| 61 | PEG | DA | 3199 | - | - | 0/4/4/4 | 0/0/0/0 |
| 61 | PEG | DA | 3200 | - | - | 0/4/4/4 | 0/0/0/0 |
| 61 | PEG | DA | 3201 | - | - | 0/4/4/4 | 0/0/0/0 |
| 65 | ACY | DA | 3202 | - | - | 0/0/0/0 | 0/0/0/0 |
| 63 | 1PE | DA | 3203 | - | - | 0/13/13/13 | 0/0/0/0 |
| 64 | PGE | DA | 3204 | - | - | 0/7/7/7 | 0/0/0/0 |
| 58 | MPD | DA | 3205 | - | - | 0/5/5/5 | 0/0/0/0 |
| 59 | PUT | DA | 3206 | - | - | 0/3/3/3 | 0/0/0/0 |
| 62 | SPD | DA | 3207 | - | - | 0/7/7/7 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 58 | MPD | DA | 3208 | - | - | 0/5/5/5 | 0/0/0/0 |
| 66 | EDO | DA | 3209 | - | - | 0/1/1/1 | 0/0/0/0 |
| 66 | EDO | DA | 3210 | - | - | 0/1/1/1 | 0/0/0/0 |
| 58 | MPD | DA | 3211 | - | - | 0/5/5/5 | 0/0/0/0 |
| 67 | GUN | DA | 3212 | - | - | 0/0/0/0 | 0/2/2/2 |
| 59 | PUT | DA | 3213 | - | - | 0/3/3/3 | 0/0/0/0 |
| 59 | PUT | DA | 3214 | - | - | 0/3/3/3 | 0/0/0/0 |
| 64 | PGE | DA | 3215 | - | - | 0/7/7/7 | 0/0/0/0 |
| 66 | EDO | DA | 3216 | - | - | 0/1/1/1 | 0/0/0/0 |
| 57 | PG4 | DA | 3217 | - | - | 0/10/10/10 | 0/0/0/0 |
| 64 | PGE | DA | 3218 | - | - | 0/7/7/7 | 0/0/0/0 |
| 61 | PEG | DA | 3219 | - | - | 0/4/4/4 | 0/0/0/0 |
| 59 | PUT | DA | 3220 | - | - | 0/3/3/3 | 0/0/0/0 |
| 68 | TRS | DA | 3221 | - | - | 0/9/9/9 | 0/0/0/0 |
| 59 | PUT | DA | 3222 | - | - | 0/3/3/3 | 0/0/0/0 |
| 59 | PUT | DA | 3223 | - | - | 0/3/3/3 | 0/0/0/0 |
| 59 | PUT | DA | 3224 | - | - | 0/3/3/3 | 0/0/0/0 |
| 62 | SPD | DA | 3225 | - | - | 0/7/7/7 | 0/0/0/0 |
| 64 | PGE | DA | 3226 | - | - | 0/7/7/7 | 0/0/0/0 |
| 61 | PEG | DA | 3227 | - | - | 0/4/4/4 | 0/0/0/0 |
| 61 | PEG | DA | 3228 | - | - | 0/4/4/4 | 0/0/0/0 |
| 66 | EDO | DB | 210 | - | - | 0/1/1/1 | 0/0/0/0 |
| 66 | EDO | DB | 211 | - | - | 0/1/1/1 | 0/0/0/0 |
| 66 | EDO | DB | 212 | - | - | 0/1/1/1 | 0/0/0/0 |
| 58 | MPD | DE | 301 | - | - | 0/5/5/5 | 0/0/0/0 |
| 58 | MPD | DE | 302 | - | - | 0/5/5/5 | 0/0/0/0 |
| 58 | MPD | DK | 201 | - | - | 0/5/5/5 | 0/0/0/0 |
| 61 | PEG | DL | 201 | - | - | 0/4/4/4 | 0/0/0/0 |
| 59 | PUT | DM | 201 | - | - | 0/3/3/3 | 0/0/0/0 |
| 58 | MPD | DN | 201 | - | - | 0/5/5/5 | 0/0/0/0 |
| 61 | PEG | DP | 201 | - | - | 0/4/4/4 | 0/0/0/0 |
| 61 | PEG | DQ | 201 | - | - | 0/4/4/4 | 0/0/0/0 |
| 57 | PG4 | DQ | 202 | - | - | 0/10/10/10 | 0/0/0/0 |
| 57 | PG4 | DR | 202 | - | - | 0/10/10/10 | 0/0/0/0 |
| 66 | EDO | DR | 203 | - | - | 0/1/1/1 | 0/0/0/0 |
| 64 | PGE | DS | 201 | - | - | 0/7/7/7 | 0/0/0/0 |
| 57 | PG4 | DS | 202 | - | - | 0/10/10/10 | 0/0/0/0 |
| 58 | MPD | DS | 203 | - | - | 0/5/5/5 | 0/0/0/0 |
| 58 | MPD | DT | 201 | - | - | 0/5/5/5 | 0/0/0/0 |
| 58 | MPD | DT | 202 | - | - | 0/5/5/5 | 0/0/0/0 |
| 64 | PGE | DU | 101 | - | - | 0/7/7/7 | 0/0/0/0 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 65 | DA | 3202 | ACY | CH3-C | 2.23 | 1.51 | 1.48 |
| 65 | DA | 3191 | ACY | CH3-C | 2.32 | 1.52 | 1.48 |
| 65 | DA | 3196 | ACY | CH3-C | 3.25 | 1.53 | 1.48 |
| 67 | DA | 3212 | GUN | C5-C4 | 3.48 | 1.48 | 1.40 |
| 67 | DA | 3212 | GUN | C6-C5 | 4.78 | 1.50 | 1.41 |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 67 | DA | 3212 | GUN | C4-C5-N7 | -3.97 | 105.82 | 109.48 |
| 67 | DA | 3212 | GUN | C6-C5-C4 | -3.47 | 116.75 | 120.90 |
| 67 | DA | 3212 | GUN | C5-C6-N1 | -3.25 | 119.14 | 123.59 |
| 58 | DA | 3192 | MPD | CM-C2-C1 | -3.22 | 103.22 | 110.24 |
| 67 | DA | 3212 | GUN | N3-C2-N1 | -3.07 | 122.78 | 127.44 |
| 62 | DA | 3225 | SPD | C7-C8-C9 | -2.22 | 105.22 | 114.31 |
| 58 | DA | 3211 | MPD | CM-C2-C1 | -2.17 | 105.52 | 110.24 |
| 68 | DA | 3221 | TRS | C3-C-C1 | 2.00 | 115.12 | 110.78 |
| 58 | DA | 3205 | MPD | CM-C2-C1 | 2.86 | 116.47 | 110.24 |
| 67 | DA | 3212 | GUN | C6-N1-C2 | 3.96 | 121.44 | 115.94 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

42 monomers are involved in 92 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 57 | AA | 1670 | PG4 | 1 | 0 |
| 59 | AA | 1673 | PUT | 1 | 0 |
| 57 | BA | 1642 | PG4 | 2 | 0 |
| 61 | D3 | 102 | PEG | 5 | 0 |
| 62 | DA | 3183 | SPD | 1 | 0 |
| 63 | DA | 3185 | 1PE | 1 | 0 |
| 62 | DA | 3187 | SPD | 1 | 0 |
| 59 | DA | 3189 | PUT | 1 | 0 |
| 58 | DA | 3190 | MPD | 1 | 0 |
| 57 | DA | 3193 | PG4 | 7 | 0 |
| 66 | DA | 3194 | EDO | 3 | 0 |
| 59 | DA | 3195 | PUT | 3 | 0 |
| 66 | DA | 3197 | EDO | 1 | 0 |
| 66 | DA | 3198 | EDO | 3 | 0 |
| 61 | DA | 3200 | PEG | 1 | 0 |
| 61 | DA | 3201 | PEG | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 65 | DA | 3202 | ACY | 1 | 0 |
| 63 | DA | 3203 | 1PE | 3 | 0 |
| 64 | DA | 3204 | PGE | 2 | 0 |
| 58 | DA | 3205 | MPD | 3 | 0 |
| 66 | DA | 3209 | EDO | 1 | 0 |
| 66 | DA | 3210 | EDO | 3 | 0 |
| 58 | DA | 3211 | MPD | 1 | 0 |
| 67 | DA | 3212 | GUN | 1 | 0 |
| 59 | DA | 3213 | PUT | 1 | 0 |
| 59 | DA | 3214 | PUT | 2 | 0 |
| 57 | DA | 3217 | PG4 | 1 | 0 |
| 64 | DA | 3218 | PGE | 1 | 0 |
| 59 | DA | 3220 | PUT | 1 | 0 |
| 59 | DA | 3222 | PUT | 2 | 0 |
| 59 | DA | 3223 | PUT | 4 | 0 |
| 59 | DA | 3224 | PUT | 2 | 0 |
| 62 | DA | 3225 | SPD | 5 | 0 |
| 61 | DA | 3227 | PEG | 1 | 0 |
| 66 | DB | 212 | EDO | 1 | 0 |
| 58 | DN | 201 | MPD | 6 | 0 |
| 61 | DP | 201 | PEG | 4 | 0 |
| 61 | DQ | 201 | PEG | 1 | 0 |
| 57 | DQ | 202 | PG4 | 3 | 0 |
| 57 | DR | 202 | PG4 | 10 | 0 |
| 57 | DS | 202 | PG4 | 2 | 0 |
| 64 | DU | 101 | PGE | 1 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1 | AA | 1523/1534 (99%) | 0.36 | 104 (6%) 20 28 | 50, 82, 132, 172 | 0 |
| 1 | BA | 1522/1534 (99%) | 1.27 | 317 (20%) 1 1 | 64, 105, 192, 222 | 0 |
| 2 | AB | 224/224 (100%) | 3.08 | 141 (62%) 0 0 | 74, 117, 124, 132 | 0 |
| 2 | BB | 224/224 (100%) | 3.93 | 163 (72%) 0 0 | 74, 114, 123, 130 | 0 |
| 3 | AC | 206/206 (100%) | 1.29 | 46 (22%) 1 1 | 77, 88, 100, 105 | 0 |
| 3 | BC | 206/206 (100%) | 3.35 | 140 (67%) 0 0 | 99, 117, 150, 166 | 0 |
| 4 | AD | 205/205 (100%) | 0.88 | 23 (11%) 7 9 | 70, 91, 116, 125 | 0 |
| 4 | BD | 205/205 (100%) | 1.02 | 15 (7%) 18 24 | 64, 76, 86, 91 | 0 |
| 5 | AE | 155/155 (100%) | 1.04 | 26 (16%) 2 3 | 68, 79, 89, 95 | 0 |
| 5 | BE | 150/155 (96%) | 1.82 | 50 (33%) 0 1 | 77, 91, 103, 114 | 0 |
| 6 | AF | 106/106 (100%) | 0.83 | 13 (12%) 5 7 | 65, 92, 100, 102 | 0 |
| 6 | BF | 100/106 (94%) | 2.60 | 53 (53%) 0 0 | 92, 104, 113, 117 | 0 |
| 7 | AG | 151/151 (100%) | 2.44 | 66 (43%) 0 0 | 90, 117, 127, 132 | 0 |
| 7 | BG | 151/151 (100%) | 7.00 | 140 (92%) 0 0 | 111, 153, 177, 185 | 0 |
| 8 | AH | 129/129 (100%) | 0.89 | 15 (11%) 6 9 | 69, 82, 95, 103 | 0 |
| 8 | BH | 129/129 (100%) | 1.71 | 40 (31%) 1 1 | 72, 111, 132, 139 | 0 |
| 9 | AI | 127/127 (100%) | 2.69 | 66 (51%) 0 0 | 81, 111, 124, 130 | 0 |
| 9 | BI | 127/127 (100%) | 5.37 | 105 (82%) 0 0 | 130, 152, 171, 177 | 0 |
| 10 | AJ | 99/99 (100%) | 2.11 | 43 (43%) 0 0 | 60, 70, 76, 77 | 0 |
| 10 | BJ | 98/99 (98%) | 5.62 | 84 (85%) 0 0 | 69, 76, 80, 81 | 0 |
| 11 | AK | 117/117 (100%) | 1.68 | 43 (36%) 0 0 | 60, 90, 104, 108 | 0 |
| 11 | BK | 117/117 (100%) | 2.22 | 54 (46%) 0 0 | 75, 102, 115, 118 | 0 |
| 12 | AL | 122/123 (99%) | 0.54 | 5 (4%) 41 50 | 55, 67, 77, 88 | 0 |
| 12 | BL | 122/123 (99%) | 1.39 | 29 (23%) 1 1 | 72, 84, 92, 94 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å²) | | Q<0.9 | |
|-----|-------|-----------------|--------|-----------|----------|-----|--------------------|---|
| 13 | AM | 114/114 (100%) | 2.63 | 57 (50%) | 0 | 0 | 84, 112, 124, 128 | 0 |
| 13 | BM | 114/114 (100%) | 8.85 | 110 (96%) | 0 | 0 | 190, 219, 233, 235 | 0 |
| 14 | AN | 100/100 (100%) | 2.25 | 36 (36%) | 0 | 0 | 80, 100, 134, 140 | 0 |
| 14 | BN | 100/100 (100%) | 7.18 | 93 (93%) | 0 | 0 | 126, 174, 220, 227 | 0 |
| 15 | AO | 88/88 (100%) | 0.81 | 10 (11%) | 7 | 9 | 69, 82, 93, 98 | 0 |
| 15 | BO | 88/88 (100%) | 1.99 | 36 (40%) | 0 | 0 | 80, 105, 118, 125 | 0 |
| 16 | AP | 82/82 (100%) | 1.59 | 17 (20%) | 1 | 1 | 70, 85, 104, 113 | 0 |
| 16 | BP | 82/82 (100%) | 3.09 | 57 (69%) | 0 | 0 | 84, 106, 122, 126 | 0 |
| 17 | AQ | 80/80 (100%) | 1.13 | 18 (22%) | 1 | 1 | 69, 83, 96, 101 | 0 |
| 17 | BQ | 80/80 (100%) | 3.40 | 54 (67%) | 0 | 0 | 89, 120, 129, 133 | 0 |
| 18 | AR | 55/55 (100%) | 1.53 | 17 (30%) | 1 | 1 | 79, 86, 96, 98 | 0 |
| 18 | BR | 55/55 (100%) | 1.34 | 12 (21%) | 1 | 1 | 83, 90, 98, 100 | 0 |
| 19 | AS | 79/79 (100%) | 2.65 | 43 (54%) | 0 | 0 | 91, 110, 123, 127 | 0 |
| 19 | BS | 79/79 (100%) | 9.48 | 71 (89%) | 0 | 0 | 199, 217, 228, 231 | 0 |
| 20 | AT | 86/86 (100%) | 1.25 | 17 (19%) | 1 | 2 | 58, 84, 101, 107 | 0 |
| 20 | BT | 85/86 (98%) | 4.38 | 67 (78%) | 0 | 0 | 107, 131, 142, 144 | 0 |
| 21 | AU | 56/56 (100%) | 2.67 | 32 (57%) | 0 | 0 | 67, 80, 103, 113 | 0 |
| 21 | BU | 56/56 (100%) | 2.00 | 24 (42%) | 0 | 0 | 65, 85, 106, 113 | 0 |
| 22 | CA | 2876/2904 (99%) | 1.56 | 670 (23%) | 1 | 1 | 77, 118, 180, 217 | 0 |
| 23 | CB | 118/120 (98%) | 1.88 | 48 (40%) | 0 | 0 | 108, 157, 167, 168 | 0 |
| 23 | DB | 120/120 (100%) | 0.23 | 0 | 100 | 100 | 37, 58, 73, 81 | 0 |
| 24 | CC | 271/271 (100%) | 2.14 | 132 (48%) | 0 | 0 | 83, 107, 126, 131 | 0 |
| 24 | DC | 271/271 (100%) | 1.41 | 64 (23%) | 1 | 1 | 35, 59, 71, 78 | 0 |
| 25 | CD | 209/209 (100%) | 2.78 | 122 (58%) | 0 | 0 | 87, 108, 121, 126 | 0 |
| 26 | CE | 201/201 (100%) | 4.72 | 154 (76%) | 0 | 0 | 90, 157, 187, 196 | 0 |
| 26 | DE | 201/201 (100%) | 0.78 | 26 (12%) | 5 | 6 | 33, 57, 72, 78 | 0 |
| 27 | CF | 177/177 (100%) | 8.81 | 171 (96%) | 0 | 0 | 167, 172, 175, 176 | 0 |
| 27 | DF | 177/177 (100%) | 0.97 | 19 (10%) | 8 | 11 | 58, 75, 91, 94 | 0 |
| 28 | CG | 176/176 (100%) | 5.65 | 155 (88%) | 0 | 0 | 108, 120, 130, 134 | 0 |
| 28 | DG | 176/176 (100%) | 0.63 | 14 (7%) | 15 | 21 | 49, 62, 71, 75 | 0 |
| 29 | CH | 149/149 (100%) | 4.19 | 117 (78%) | 0 | 0 | 96, 121, 141, 223 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|----------------|-----------------------|-------|
| 29 | DH | 149/149 (100%) | 4.08 | 104 (69%) 0 0 | 65, 128, 133, 154 | 0 |
| 30 | CJ | 134/134 (100%) | 13.06 | 134 (100%) 0 0 | 202, 219, 225, 228 | 0 |
| 30 | DJ | 134/134 (100%) | 10.29 | 131 (97%) 0 0 | 155, 183, 202, 208 | 0 |
| 31 | CK | 142/142 (100%) | 2.49 | 82 (57%) 0 0 | 98, 110, 115, 120 | 0 |
| 31 | DK | 142/142 (100%) | 1.06 | 25 (17%) 2 3 | 33, 41, 51, 60 | 0 |
| 32 | CL | 122/123 (99%) | 2.30 | 54 (44%) 0 0 | 94, 107, 113, 114 | 0 |
| 32 | DL | 123/123 (100%) | 0.75 | 8 (6%) 22 29 | 37, 48, 59, 68 | 0 |
| 33 | CM | 144/144 (100%) | 4.28 | 119 (82%) 0 0 | 100, 137, 162, 166 | 0 |
| 33 | DM | 144/144 (100%) | 1.12 | 32 (22%) 1 1 | 28, 53, 69, 73 | 0 |
| 34 | CN | 135/136 (99%) | 2.29 | 59 (43%) 0 0 | 95, 122, 142, 150 | 0 |
| 34 | DN | 135/136 (99%) | 0.61 | 6 (4%) 38 47 | 36, 44, 57, 63 | 0 |
| 35 | CO | 120/125 (96%) | 3.10 | 79 (65%) 0 0 | 103, 120, 137, 142 | 0 |
| 35 | DO | 125/125 (100%) | 1.30 | 27 (21%) 1 1 | 35, 44, 60, 69 | 0 |
| 36 | CP | 116/117 (99%) | 6.03 | 107 (92%) 0 0 | 146, 155, 162, 164 | 0 |
| 36 | DP | 117/117 (100%) | 0.40 | 2 (1%) 73 78 | 49, 59, 69, 73 | 0 |
| 37 | CQ | 114/114 (100%) | 2.92 | 71 (62%) 0 0 | 110, 116, 124, 131 | 0 |
| 37 | DQ | 114/114 (100%) | 0.92 | 14 (12%) 5 7 | 40, 52, 63, 73 | 0 |
| 38 | CR | 117/117 (100%) | 2.60 | 71 (60%) 0 0 | 100, 115, 126, 128 | 0 |
| 38 | DR | 117/117 (100%) | 1.51 | 36 (30%) 1 1 | 30, 40, 49, 64 | 0 |
| 39 | CS | 103/103 (100%) | 3.69 | 73 (70%) 0 0 | 103, 125, 133, 137 | 0 |
| 39 | DS | 103/103 (100%) | 0.88 | 11 (10%) 8 11 | 29, 48, 59, 73 | 0 |
| 40 | CT | 110/110 (100%) | 3.29 | 78 (70%) 0 0 | 91, 121, 146, 150 | 0 |
| 40 | DT | 110/110 (100%) | 1.22 | 12 (10%) 7 10 | 33, 39, 52, 68 | 0 |
| 41 | CU | 93/93 (100%) | 5.90 | 82 (88%) 0 0 | 117, 149, 169, 176 | 0 |
| 41 | DU | 93/93 (100%) | 0.72 | 7 (7%) 17 23 | 41, 57, 76, 83 | 0 |
| 42 | CV | 102/102 (100%) | 7.77 | 96 (94%) 0 0 | 151, 176, 205, 210 | 0 |
| 42 | DV | 102/102 (100%) | 0.49 | 4 (3%) 43 52 | 48, 60, 69, 80 | 0 |
| 43 | CW | 94/94 (100%) | 3.69 | 64 (68%) 0 0 | 129, 148, 161, 165 | 0 |
| 43 | DW | 94/94 (100%) | 0.48 | 3 (3%) 51 60 | 40, 54, 65, 71 | 0 |
| 44 | CX | 75/76 (98%) | 3.57 | 51 (68%) 0 0 | 109, 118, 122, 126 | 0 |
| 44 | DX | 76/76 (100%) | 1.18 | 14 (18%) 2 2 | 36, 46, 59, 65 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|--------|
| 45 | CY | 77/77 (100%) | 2.63 | 41 (53%) 0 0 | 99, 116, 133, 135 | 0 |
| 45 | DY | 77/77 (100%) | 0.75 | 4 (5%) 31 39 | 42, 59, 73, 78 | 0 |
| 46 | CZ | 62/62 (100%) | 5.42 | 57 (91%) 0 0 | 158, 174, 193, 199 | 0 |
| 46 | DZ | 62/62 (100%) | 0.59 | 4 (6%) 22 29 | 56, 66, 81, 82 | 0 |
| 47 | C0 | 58/58 (100%) | 2.29 | 23 (39%) 0 0 | 119, 130, 142, 143 | 0 |
| 47 | D0 | 58/58 (100%) | 1.27 | 11 (18%) 2 2 | 35, 42, 53, 56 | 0 |
| 48 | C1 | 56/56 (100%) | 3.51 | 44 (78%) 0 0 | 92, 123, 140, 144 | 0 |
| 48 | D1 | 56/56 (100%) | 1.38 | 17 (30%) 1 1 | 27, 44, 58, 64 | 0 |
| 49 | C2 | 50/51 (98%) | 3.84 | 41 (82%) 0 0 | 113, 122, 128, 132 | 0 |
| 49 | D2 | 51/51 (100%) | 0.90 | 6 (11%) 6 8 | 50, 59, 66, 67 | 0 |
| 50 | C3 | 46/46 (100%) | 3.46 | 35 (76%) 0 0 | 95, 108, 115, 117 | 0 |
| 50 | D3 | 46/46 (100%) | 1.36 | 5 (10%) 7 10 | 35, 44, 53, 62 | 0 |
| 51 | C4 | 64/64 (100%) | 3.55 | 47 (73%) 0 0 | 109, 119, 126, 127 | 0 |
| 51 | D4 | 64/64 (100%) | 1.82 | 23 (35%) 0 0 | 39, 45, 51, 57 | 0 |
| 52 | C5 | 38/38 (100%) | 3.25 | 25 (65%) 0 0 | 106, 114, 120, 125 | 0 |
| 52 | D5 | 38/38 (100%) | 0.68 | 1 (2%) 59 66 | 42, 48, 58, 63 | 0 |
| 53 | DA | 2873/2903 (98%) | 0.88 | 277 (9%) 10 14 | 30, 49, 130, 199 | 0 |
| 54 | DD | 208/209 (99%) | 1.24 | 51 (24%) 1 1 | 29, 44, 58, 63 | 0 |
| 55 | DI | 135/135 (100%) | 5.77 | 119 (88%) 0 0 | 89, 123, 152, 159 | 1 (0%) |
| All | All | 20634/20744 (99%) | 2.09 | 6731 (32%) 1 1 | 27, 96, 176, 235 | 1 (0%) |

All (6731) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 30 | CJ | 32 | GLY | 67.6 |
| 30 | CJ | 8 | TYR | 50.0 |
| 30 | CJ | 9 | VAL | 40.8 |
| 30 | CJ | 11 | LEU | 33.2 |
| 30 | CJ | 13 | VAL | 32.9 |
| 30 | CJ | 26 | PRO | 32.1 |
| 30 | CJ | 42 | PHE | 30.7 |
| 14 | BN | 34 | VAL | 30.5 |
| 30 | CJ | 67 | PHE | 29.2 |
| 42 | CV | 26 | LYS | 29.1 |
| 7 | BG | 62 | PHE | 29.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 30 | CJ | 31 | GLN | 28.9 |
| 30 | CJ | 69 | PHE | 28.4 |
| 14 | BN | 21 | PHE | 28.0 |
| 27 | CF | 156 | ILE | 27.1 |
| 30 | CJ | 63 | ALA | 26.3 |
| 30 | DJ | 67 | PHE | 25.6 |
| 42 | CV | 12 | ILE | 24.7 |
| 30 | DJ | 99 | GLY | 24.5 |
| 30 | CJ | 62 | TYR | 24.4 |
| 30 | DJ | 80 | LEU | 24.4 |
| 27 | CF | 76 | GLY | 24.3 |
| 30 | CJ | 99 | GLY | 23.5 |
| 42 | CV | 25 | VAL | 23.2 |
| 30 | CJ | 80 | LEU | 23.2 |
| 19 | BS | 68 | GLY | 23.1 |
| 19 | BS | 74 | PHE | 22.6 |
| 9 | BI | 38 | TYR | 22.4 |
| 41 | CU | 1 | MET | 22.2 |
| 30 | CJ | 35 | ILE | 21.8 |
| 13 | BM | 84 | GLY | 21.8 |
| 42 | CV | 50 | PRO | 21.7 |
| 55 | DI | 123 | ILE | 21.4 |
| 30 | DJ | 53 | LEU | 21.4 |
| 13 | BM | 40 | ALA | 21.3 |
| 13 | BM | 75 | MET | 21.2 |
| 30 | CJ | 27 | ALA | 21.0 |
| 13 | BM | 85 | CYS | 21.0 |
| 46 | CZ | 11 | VAL | 21.0 |
| 30 | DJ | 49 | ILE | 20.8 |
| 43 | CW | 94 | ALA | 20.8 |
| 19 | BS | 15 | LEU | 20.7 |
| 7 | BG | 66 | LEU | 20.5 |
| 19 | BS | 12 | ASP | 20.2 |
| 30 | CJ | 17 | MET | 20.1 |
| 30 | DJ | 85 | GLY | 20.0 |
| 30 | DJ | 98 | VAL | 19.9 |
| 27 | CF | 97 | TRP | 19.8 |
| 7 | BG | 87 | VAL | 19.8 |
| 30 | DJ | 106 | LEU | 19.8 |
| 27 | CF | 152 | LEU | 19.6 |
| 30 | DJ | 100 | LYS | 19.5 |
| 13 | BM | 30 | SER | 19.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 13 | BM | 80 | LEU | 19.4 |
| 30 | CJ | 33 | VAL | 19.2 |
| 7 | BG | 51 | ALA | 19.0 |
| 30 | CJ | 44 | ALA | 19.0 |
| 19 | BS | 66 | MET | 19.0 |
| 30 | DJ | 40 | LYS | 19.0 |
| 30 | CJ | 21 | SER | 19.0 |
| 30 | DJ | 48 | SER | 18.9 |
| 51 | C4 | 21 | GLY | 18.8 |
| 14 | BN | 31 | ILE | 18.8 |
| 42 | CV | 51 | ALA | 18.8 |
| 30 | DJ | 87 | LYS | 18.7 |
| 30 | CJ | 56 | PRO | 18.7 |
| 30 | CJ | 59 | ILE | 18.7 |
| 14 | BN | 33 | ASP | 18.6 |
| 42 | CV | 29 | LEU | 18.5 |
| 30 | DJ | 138 | LEU | 18.4 |
| 30 | CJ | 22 | PRO | 18.3 |
| 2 | BB | 135 | LEU | 18.2 |
| 42 | CV | 28 | VAL | 18.2 |
| 55 | DI | 131 | THR | 18.2 |
| 19 | BS | 67 | VAL | 18.2 |
| 19 | BS | 46 | GLY | 18.1 |
| 30 | CJ | 75 | PRO | 18.0 |
| 13 | BM | 5 | ALA | 18.0 |
| 14 | BN | 74 | LEU | 18.0 |
| 30 | DJ | 96 | ASP | 17.9 |
| 30 | CJ | 10 | LYS | 17.8 |
| 14 | BN | 25 | ALA | 17.8 |
| 42 | CV | 39 | ILE | 17.7 |
| 30 | CJ | 12 | GLN | 17.7 |
| 9 | BI | 58 | VAL | 17.7 |
| 9 | BI | 40 | GLY | 17.5 |
| 30 | DJ | 94 | ASN | 17.5 |
| 30 | CJ | 58 | VAL | 17.5 |
| 30 | CJ | 57 | VAL | 17.4 |
| 42 | CV | 62 | GLU | 17.4 |
| 26 | CE | 119 | ILE | 17.4 |
| 27 | CF | 155 | THR | 17.3 |
| 27 | CF | 117 | LEU | 17.2 |
| 7 | BG | 59 | LEU | 17.2 |
| 14 | BN | 36 | ALA | 17.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 30 | CJ | 20 | PRO | 17.1 |
| 55 | DI | 84 | TYR | 17.1 |
| 14 | BN | 30 | ILE | 17.0 |
| 14 | BN | 43 | ASN | 17.0 |
| 30 | CJ | 73 | THR | 17.0 |
| 30 | DJ | 88 | SER | 16.9 |
| 30 | DJ | 114 | ALA | 16.9 |
| 27 | CF | 120 | LYS | 16.9 |
| 14 | BN | 42 | TRP | 16.9 |
| 13 | BM | 109 | ARG | 16.8 |
| 27 | CF | 100 | PHE | 16.8 |
| 30 | CJ | 30 | GLN | 16.8 |
| 13 | BM | 106 | ALA | 16.8 |
| 30 | CJ | 29 | GLY | 16.8 |
| 7 | BG | 152 | ALA | 16.8 |
| 42 | CV | 87 | PHE | 16.7 |
| 20 | BT | 4 | ILE | 16.7 |
| 14 | AN | 21 | PHE | 16.6 |
| 10 | BJ | 77 | VAL | 16.5 |
| 19 | BS | 11 | ILE | 16.5 |
| 30 | CJ | 60 | THR | 16.5 |
| 19 | BS | 22 | ALA | 16.5 |
| 27 | CF | 4 | LEU | 16.4 |
| 14 | BN | 57 | PRO | 16.4 |
| 30 | DJ | 110 | ALA | 16.4 |
| 13 | BM | 6 | GLY | 16.3 |
| 13 | BM | 96 | PRO | 16.3 |
| 30 | CJ | 76 | ALA | 16.2 |
| 26 | CE | 158 | PHE | 16.2 |
| 30 | CJ | 139 | VAL | 16.0 |
| 28 | CG | 168 | VAL | 16.0 |
| 27 | CF | 169 | LEU | 16.0 |
| 27 | CF | 58 | ALA | 15.9 |
| 27 | CF | 28 | VAL | 15.9 |
| 27 | CF | 113 | ASP | 15.8 |
| 43 | CW | 57 | TYR | 15.8 |
| 27 | CF | 159 | THR | 15.7 |
| 30 | CJ | 64 | ASP | 15.7 |
| 27 | CF | 106 | ILE | 15.7 |
| 7 | BG | 134 | ALA | 15.7 |
| 28 | CG | 40 | ALA | 15.7 |
| 27 | CF | 55 | ALA | 15.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 36 | CP | 58 | ILE | 15.6 |
| 30 | DJ | 76 | ALA | 15.6 |
| 30 | DJ | 89 | GLY | 15.6 |
| 19 | BS | 61 | PHE | 15.6 |
| 30 | CJ | 61 | VAL | 15.5 |
| 30 | DJ | 38 | PHE | 15.5 |
| 55 | DI | 106 | PHE | 15.5 |
| 55 | DI | 129 | LEU | 15.5 |
| 13 | BM | 32 | ALA | 15.5 |
| 30 | DJ | 52 | GLY | 15.4 |
| 30 | DJ | 139 | VAL | 15.4 |
| 30 | CJ | 34 | ASN | 15.4 |
| 22 | CA | 138 | U | 15.4 |
| 30 | CJ | 68 | THR | 15.4 |
| 30 | DJ | 42 | PHE | 15.4 |
| 30 | DJ | 54 | PRO | 15.3 |
| 9 | BI | 47 | VAL | 15.3 |
| 42 | CV | 13 | VAL | 15.3 |
| 9 | BI | 128 | SER | 15.2 |
| 19 | BS | 58 | VAL | 15.2 |
| 28 | CG | 52 | PHE | 15.2 |
| 30 | CJ | 25 | GLY | 15.2 |
| 13 | BM | 39 | ILE | 15.0 |
| 42 | CV | 36 | VAL | 15.0 |
| 14 | BN | 28 | LYS | 14.9 |
| 27 | CF | 57 | LEU | 14.9 |
| 7 | BG | 141 | VAL | 14.9 |
| 27 | CF | 116 | GLY | 14.9 |
| 14 | BN | 58 | SER | 14.9 |
| 19 | BS | 27 | ASP | 14.8 |
| 42 | CV | 30 | SER | 14.8 |
| 55 | DI | 121 | SER | 14.7 |
| 2 | BB | 40 | ILE | 14.7 |
| 19 | BS | 60 | VAL | 14.7 |
| 42 | CV | 52 | LEU | 14.7 |
| 7 | BG | 98 | ALA | 14.6 |
| 42 | CV | 37 | GLU | 14.5 |
| 13 | BM | 51 | GLY | 14.5 |
| 27 | CF | 40 | VAL | 14.5 |
| 30 | CJ | 140 | VAL | 14.5 |
| 27 | CF | 136 | ILE | 14.4 |
| 26 | CE | 128 | ALA | 14.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 55 | DI | 117 | LEU | 14.4 |
| 30 | DJ | 33 | VAL | 14.4 |
| 27 | CF | 176 | PRO | 14.4 |
| 27 | CF | 172 | ALA | 14.4 |
| 29 | DH | 74 | ALA | 14.4 |
| 27 | CF | 32 | GLU | 14.4 |
| 30 | DJ | 13 | VAL | 14.4 |
| 20 | BT | 79 | LEU | 14.3 |
| 30 | CJ | 38 | PHE | 14.3 |
| 19 | BS | 38 | SER | 14.3 |
| 39 | CS | 103 | ALA | 14.3 |
| 30 | DJ | 68 | THR | 14.3 |
| 30 | DJ | 79 | LEU | 14.3 |
| 13 | BM | 77 | ILE | 14.3 |
| 26 | CE | 164 | LEU | 14.3 |
| 55 | DI | 130 | PRO | 14.3 |
| 28 | CG | 10 | VAL | 14.3 |
| 26 | CE | 131 | THR | 14.3 |
| 41 | CU | 83 | ALA | 14.2 |
| 19 | BS | 26 | GLY | 14.2 |
| 30 | CJ | 23 | PRO | 14.2 |
| 7 | BG | 5 | ARG | 14.1 |
| 26 | CE | 12 | LEU | 14.1 |
| 30 | DJ | 22 | PRO | 14.1 |
| 30 | DJ | 69 | PHE | 14.1 |
| 22 | CA | 1067 | A | 14.1 |
| 33 | CM | 92 | LEU | 14.1 |
| 13 | BM | 28 | THR | 14.1 |
| 26 | CE | 127 | GLU | 14.1 |
| 27 | CF | 54 | ALA | 14.1 |
| 19 | BS | 39 | THR | 14.1 |
| 46 | CZ | 6 | LEU | 14.1 |
| 36 | CP | 59 | ALA | 14.0 |
| 7 | BG | 79 | ARG | 14.0 |
| 30 | DJ | 55 | ILE | 14.0 |
| 13 | BM | 83 | LEU | 13.9 |
| 7 | BG | 133 | THR | 13.9 |
| 22 | CA | 1068 | G | 13.9 |
| 30 | DJ | 140 | VAL | 13.9 |
| 27 | CF | 128 | TYR | 13.9 |
| 19 | BS | 25 | SER | 13.9 |
| 30 | DJ | 36 | MET | 13.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | DJ | 103 | ARG | 13.9 |
| 7 | BG | 50 | LEU | 13.8 |
| 27 | CF | 87 | CYS | 13.8 |
| 42 | CV | 75 | ALA | 13.8 |
| 7 | BG | 46 | ALA | 13.7 |
| 19 | BS | 69 | HIS | 13.7 |
| 30 | DJ | 93 | PRO | 13.7 |
| 13 | BM | 45 | ILE | 13.7 |
| 30 | DJ | 9 | VAL | 13.7 |
| 27 | CF | 79 | ILE | 13.7 |
| 14 | BN | 18 | ASP | 13.7 |
| 30 | DJ | 133 | ALA | 13.6 |
| 22 | CA | 1175 | A | 13.6 |
| 9 | BI | 59 | GLU | 13.6 |
| 22 | CA | 613 | A | 13.6 |
| 42 | CV | 31 | SER | 13.6 |
| 30 | DJ | 115 | ALA | 13.6 |
| 30 | CJ | 70 | VAL | 13.6 |
| 41 | CU | 55 | VAL | 13.6 |
| 13 | BM | 2 | ALA | 13.5 |
| 27 | CF | 34 | ILE | 13.5 |
| 30 | DJ | 86 | ILE | 13.5 |
| 39 | CS | 27 | ILE | 13.5 |
| 27 | CF | 22 | TYR | 13.5 |
| 42 | CV | 20 | GLY | 13.5 |
| 9 | BI | 37 | GLN | 13.5 |
| 28 | CG | 102 | VAL | 13.4 |
| 27 | CF | 65 | PRO | 13.4 |
| 30 | DJ | 116 | ASP | 13.4 |
| 7 | BG | 65 | ALA | 13.3 |
| 9 | AI | 130 | ARG | 13.3 |
| 27 | CF | 13 | VAL | 13.3 |
| 29 | CH | 13 | GLY | 13.3 |
| 30 | CJ | 36 | MET | 13.3 |
| 19 | BS | 42 | PRO | 13.3 |
| 30 | CJ | 14 | ALA | 13.2 |
| 30 | CJ | 41 | ALA | 13.2 |
| 30 | DJ | 135 | SER | 13.2 |
| 19 | BS | 13 | LEU | 13.1 |
| 10 | BJ | 26 | VAL | 13.0 |
| 27 | CF | 8 | TYR | 13.0 |
| 27 | CF | 12 | VAL | 13.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 27 | CF | 154 | ILE | 12.9 |
| 30 | CJ | 109 | ILE | 12.9 |
| 3 | BC | 29 | PHE | 12.9 |
| 55 | DI | 128 | THR | 12.9 |
| 32 | CL | 111 | LYS | 12.9 |
| 3 | BC | 193 | TYR | 12.9 |
| 13 | BM | 31 | LYS | 12.9 |
| 10 | BJ | 100 | ILE | 12.9 |
| 10 | BJ | 87 | LEU | 12.9 |
| 41 | CU | 45 | ALA | 12.9 |
| 27 | CF | 7 | TYR | 12.9 |
| 19 | BS | 30 | PRO | 12.8 |
| 30 | CJ | 65 | ARG | 12.8 |
| 30 | CJ | 120 | ALA | 12.8 |
| 13 | BM | 22 | ILE | 12.8 |
| 30 | DJ | 28 | LEU | 12.8 |
| 36 | CP | 40 | ILE | 12.7 |
| 26 | CE | 121 | VAL | 12.7 |
| 14 | BN | 8 | ALA | 12.7 |
| 30 | DJ | 47 | ASP | 12.7 |
| 30 | CJ | 51 | LYS | 12.7 |
| 26 | CE | 13 | THR | 12.6 |
| 33 | CM | 89 | VAL | 12.6 |
| 41 | CU | 53 | VAL | 12.6 |
| 46 | CZ | 33 | ALA | 12.6 |
| 19 | BS | 65 | GLU | 12.6 |
| 30 | CJ | 71 | THR | 12.6 |
| 19 | BS | 59 | PRO | 12.5 |
| 30 | DJ | 39 | CYS | 12.5 |
| 13 | BM | 10 | PRO | 12.5 |
| 19 | BS | 29 | LYS | 12.5 |
| 30 | DJ | 51 | LYS | 12.5 |
| 30 | CJ | 119 | GLY | 12.5 |
| 7 | BG | 52 | GLN | 12.5 |
| 27 | CF | 59 | ALA | 12.5 |
| 28 | CG | 157 | TYR | 12.5 |
| 3 | BC | 28 | GLU | 12.4 |
| 13 | BM | 113 | ARG | 12.4 |
| 30 | CJ | 87 | LYS | 12.4 |
| 27 | CF | 93 | GLY | 12.4 |
| 27 | CF | 75 | ALA | 12.3 |
| 26 | CE | 33 | VAL | 12.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 27 | CF | 114 | PHE | 12.3 |
| 42 | CV | 76 | ALA | 12.3 |
| 30 | DJ | 120 | ALA | 12.3 |
| 39 | CS | 51 | VAL | 12.3 |
| 30 | CJ | 110 | ALA | 12.3 |
| 30 | CJ | 138 | LEU | 12.3 |
| 29 | CH | 139 | PHE | 12.2 |
| 2 | AB | 136 | MET | 12.2 |
| 30 | DJ | 58 | VAL | 12.2 |
| 10 | BJ | 86 | ALA | 12.2 |
| 7 | BG | 27 | VAL | 12.2 |
| 2 | BB | 67 | ILE | 12.2 |
| 39 | CS | 50 | GLY | 12.2 |
| 26 | CE | 126 | VAL | 12.2 |
| 1 | BA | 1032 | G | 12.2 |
| 28 | CG | 83 | PHE | 12.1 |
| 43 | CW | 23 | ALA | 12.1 |
| 22 | CA | 1093 | G | 12.1 |
| 28 | CG | 33 | LEU | 12.1 |
| 29 | CH | 15 | LEU | 12.1 |
| 13 | BM | 36 | ALA | 12.1 |
| 9 | BI | 71 | GLY | 12.1 |
| 42 | CV | 32 | GLY | 12.0 |
| 30 | DJ | 137 | GLY | 12.0 |
| 19 | BS | 28 | LYS | 12.0 |
| 2 | BB | 215 | GLY | 12.0 |
| 30 | DJ | 101 | ILE | 12.0 |
| 7 | AG | 52 | GLN | 12.0 |
| 55 | DI | 104 | ALA | 12.0 |
| 29 | DH | 139 | PHE | 12.0 |
| 14 | BN | 22 | ALA | 12.0 |
| 13 | BM | 108 | THR | 11.9 |
| 30 | DJ | 122 | ILE | 11.9 |
| 19 | BS | 32 | ARG | 11.9 |
| 13 | BM | 67 | GLY | 11.9 |
| 28 | CG | 11 | VAL | 11.9 |
| 19 | BS | 63 | THR | 11.8 |
| 30 | CJ | 101 | ILE | 11.8 |
| 7 | BG | 129 | GLU | 11.8 |
| 13 | AM | 33 | ILE | 11.8 |
| 36 | CP | 109 | ALA | 11.8 |
| 27 | CF | 37 | ASN | 11.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 14 | BN | 27 | LEU | 11.7 |
| 7 | BG | 45 | SER | 11.7 |
| 55 | DI | 127 | ALA | 11.7 |
| 9 | BI | 130 | ARG | 11.7 |
| 7 | BG | 75 | VAL | 11.7 |
| 33 | CM | 82 | LEU | 11.7 |
| 41 | CU | 71 | GLY | 11.7 |
| 13 | BM | 35 | ALA | 11.7 |
| 13 | BM | 46 | SER | 11.7 |
| 36 | CP | 117 | PHE | 11.6 |
| 13 | BM | 55 | THR | 11.6 |
| 30 | CJ | 98 | VAL | 11.6 |
| 41 | CU | 8 | LEU | 11.6 |
| 25 | CD | 186 | LEU | 11.6 |
| 14 | BN | 32 | SER | 11.6 |
| 27 | CF | 111 | ILE | 11.6 |
| 27 | CF | 170 | LEU | 11.6 |
| 7 | BG | 61 | ALA | 11.6 |
| 29 | CH | 104 | THR | 11.6 |
| 2 | BB | 32 | PHE | 11.5 |
| 30 | CJ | 97 | LYS | 11.5 |
| 36 | CP | 97 | PHE | 11.5 |
| 7 | BG | 49 | THR | 11.5 |
| 30 | DJ | 62 | TYR | 11.5 |
| 41 | CU | 69 | ARG | 11.5 |
| 30 | DJ | 107 | GLN | 11.5 |
| 22 | CA | 1535 | A | 11.5 |
| 36 | CP | 101 | GLY | 11.5 |
| 53 | DA | 2110 | G | 11.5 |
| 1 | BA | 211 | G | 11.5 |
| 13 | BM | 97 | VAL | 11.5 |
| 13 | BM | 65 | VAL | 11.4 |
| 41 | CU | 50 | LEU | 11.4 |
| 55 | DI | 132 | TYR | 11.4 |
| 43 | CW | 58 | SER | 11.4 |
| 7 | BG | 150 | ALA | 11.4 |
| 19 | BS | 49 | ILE | 11.4 |
| 36 | CP | 21 | LEU | 11.4 |
| 2 | BB | 64 | LYS | 11.4 |
| 9 | BI | 69 | GLY | 11.4 |
| 1 | BA | 1031 | C | 11.4 |
| 14 | BN | 35 | ASN | 11.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 27 | CF | 147 | ASP | 11.3 |
| 28 | CG | 165 | ALA | 11.3 |
| 29 | DH | 75 | LEU | 11.3 |
| 29 | DH | 126 | GLY | 11.3 |
| 14 | BN | 60 | GLN | 11.3 |
| 16 | BP | 52 | LEU | 11.3 |
| 2 | BB | 186 | ILE | 11.3 |
| 13 | BM | 4 | ILE | 11.3 |
| 7 | BG | 103 | TRP | 11.2 |
| 33 | CM | 116 | VAL | 11.2 |
| 30 | DJ | 102 | SER | 11.2 |
| 27 | CF | 143 | TYR | 11.2 |
| 3 | BC | 78 | GLY | 11.2 |
| 19 | BS | 51 | VAL | 11.2 |
| 30 | CJ | 16 | GLY | 11.2 |
| 27 | CF | 173 | PHE | 11.1 |
| 26 | CE | 15 | SER | 11.1 |
| 27 | CF | 130 | MET | 11.1 |
| 20 | BT | 36 | TYR | 11.1 |
| 9 | BI | 67 | VAL | 11.1 |
| 1 | BA | 1021 | A | 11.1 |
| 16 | BP | 47 | GLU | 11.1 |
| 16 | BP | 81 | ALA | 11.1 |
| 20 | BT | 81 | ALA | 11.1 |
| 36 | CP | 22 | GLY | 11.1 |
| 27 | CF | 83 | TYR | 11.1 |
| 19 | BS | 14 | HIS | 11.1 |
| 27 | CF | 109 | PRO | 11.1 |
| 13 | BM | 26 | GLY | 11.0 |
| 36 | CP | 19 | GLN | 11.0 |
| 30 | DJ | 44 | ALA | 11.0 |
| 7 | BG | 44 | TYR | 11.0 |
| 30 | DJ | 66 | SER | 11.0 |
| 30 | DJ | 34 | ASN | 11.0 |
| 55 | DI | 124 | ASP | 11.0 |
| 55 | DI | 136 | ILE | 11.0 |
| 48 | C1 | 34 | SER | 10.9 |
| 22 | CA | 1537 | G | 10.9 |
| 33 | CM | 90 | VAL | 10.9 |
| 30 | CJ | 114 | ALA | 10.9 |
| 30 | CJ | 106 | LEU | 10.9 |
| 30 | CJ | 43 | ASN | 10.9 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 7 | BG | 88 | PRO | 10.9 |
| 19 | BS | 40 | ILE | 10.9 |
| 30 | DJ | 41 | ALA | 10.9 |
| 7 | BG | 10 | ARG | 10.9 |
| 27 | CF | 133 | ARG | 10.9 |
| 53 | DA | 2121 | G | 10.8 |
| 27 | CF | 80 | ARG | 10.8 |
| 30 | DJ | 23 | PRO | 10.8 |
| 28 | CG | 161 | GLY | 10.8 |
| 17 | BQ | 83 | VAL | 10.8 |
| 30 | DJ | 45 | LYS | 10.8 |
| 13 | AM | 19 | LEU | 10.8 |
| 33 | CM | 144 | GLU | 10.8 |
| 28 | CG | 169 | VAL | 10.8 |
| 19 | BS | 76 | PRO | 10.7 |
| 17 | BQ | 78 | VAL | 10.7 |
| 28 | CG | 91 | GLY | 10.7 |
| 26 | CE | 183 | PHE | 10.7 |
| 41 | CU | 74 | ILE | 10.7 |
| 1 | BA | 1020 | G | 10.7 |
| 28 | CG | 150 | ALA | 10.7 |
| 27 | CF | 151 | GLY | 10.7 |
| 19 | BS | 48 | THR | 10.7 |
| 27 | CF | 38 | MET | 10.7 |
| 41 | CU | 10 | VAL | 10.7 |
| 35 | CO | 76 | VAL | 10.6 |
| 27 | CF | 104 | ILE | 10.6 |
| 10 | BJ | 20 | GLN | 10.6 |
| 13 | BM | 89 | LEU | 10.6 |
| 29 | CH | 130 | VAL | 10.6 |
| 33 | CM | 117 | THR | 10.6 |
| 27 | CF | 10 | ASP | 10.6 |
| 1 | AA | 1030 | U | 10.6 |
| 36 | CP | 103 | VAL | 10.6 |
| 27 | CF | 107 | ALA | 10.6 |
| 49 | D2 | 5 | ILE | 10.5 |
| 7 | BG | 132 | GLY | 10.5 |
| 7 | BG | 77 | SER | 10.5 |
| 27 | CF | 95 | ARG | 10.5 |
| 34 | CN | 136 | MET | 10.5 |
| 36 | CP | 4 | LYS | 10.5 |
| 29 | DH | 80 | ILE | 10.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 53 | DA | 2163 | A | 10.5 |
| 13 | BM | 23 | TYR | 10.5 |
| 13 | AM | 5 | ALA | 10.4 |
| 27 | CF | 171 | ALA | 10.4 |
| 7 | BG | 80 | VAL | 10.4 |
| 36 | CP | 39 | VAL | 10.4 |
| 51 | C4 | 58 | VAL | 10.4 |
| 27 | CF | 115 | ARG | 10.4 |
| 29 | DH | 63 | ALA | 10.4 |
| 27 | CF | 103 | LEU | 10.4 |
| 30 | DJ | 14 | ALA | 10.4 |
| 30 | DJ | 30 | GLN | 10.4 |
| 13 | BM | 61 | ALA | 10.4 |
| 6 | BF | 80 | PHE | 10.4 |
| 9 | BI | 48 | VAL | 10.4 |
| 13 | BM | 64 | VAL | 10.4 |
| 28 | CG | 92 | VAL | 10.4 |
| 13 | BM | 62 | LYS | 10.4 |
| 55 | DI | 40 | GLU | 10.4 |
| 13 | BM | 7 | ILE | 10.3 |
| 30 | CJ | 28 | LEU | 10.3 |
| 44 | CX | 32 | LEU | 10.3 |
| 55 | DI | 113 | PHE | 10.3 |
| 26 | CE | 190 | ALA | 10.3 |
| 50 | C3 | 36 | ALA | 10.3 |
| 2 | BB | 130 | THR | 10.3 |
| 36 | CP | 100 | HIS | 10.3 |
| 42 | CV | 63 | ALA | 10.3 |
| 7 | BG | 73 | VAL | 10.2 |
| 27 | CF | 112 | ARG | 10.2 |
| 33 | CM | 79 | LEU | 10.2 |
| 7 | BG | 17 | LYS | 10.2 |
| 42 | CV | 35 | ILE | 10.2 |
| 27 | CF | 68 | THR | 10.2 |
| 30 | CJ | 15 | ALA | 10.2 |
| 29 | CH | 14 | SER | 10.2 |
| 42 | CV | 40 | ASN | 10.2 |
| 14 | BN | 37 | SER | 10.2 |
| 14 | BN | 56 | SER | 10.2 |
| 12 | BL | 16 | VAL | 10.2 |
| 30 | DJ | 131 | GLY | 10.2 |
| 7 | BG | 72 | THR | 10.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 14 | BN | 41 | ARG | 10.2 |
| 7 | BG | 85 | TYR | 10.2 |
| 13 | BM | 63 | PHE | 10.2 |
| 26 | CE | 172 | ALA | 10.2 |
| 7 | BG | 8 | GLY | 10.2 |
| 30 | CJ | 96 | ASP | 10.2 |
| 25 | CD | 74 | GLU | 10.1 |
| 7 | BG | 83 | SER | 10.1 |
| 49 | C2 | 36 | LEU | 10.1 |
| 7 | BG | 15 | ASP | 10.1 |
| 28 | CG | 84 | THR | 10.1 |
| 5 | BE | 99 | ALA | 10.1 |
| 29 | CH | 10 | ALA | 10.1 |
| 10 | BJ | 99 | GLN | 10.1 |
| 27 | CF | 105 | THR | 10.1 |
| 22 | CA | 1536 | C | 10.1 |
| 27 | CF | 35 | THR | 10.1 |
| 28 | CG | 2 | SER | 10.1 |
| 27 | CF | 39 | GLY | 10.1 |
| 44 | CX | 63 | ALA | 10.1 |
| 46 | CZ | 63 | ALA | 10.1 |
| 30 | CJ | 117 | MET | 10.1 |
| 10 | AJ | 6 | ILE | 10.1 |
| 7 | BG | 64 | VAL | 10.1 |
| 42 | CV | 49 | VAL | 10.1 |
| 12 | AL | 124 | ALA | 10.0 |
| 30 | CJ | 118 | THR | 10.0 |
| 2 | AB | 117 | LEU | 10.0 |
| 53 | DA | 2168 | G | 10.0 |
| 13 | BM | 37 | ALA | 10.0 |
| 27 | CF | 45 | ALA | 10.0 |
| 7 | BG | 125 | SER | 9.9 |
| 28 | CG | 103 | ILE | 9.9 |
| 19 | BS | 23 | VAL | 9.9 |
| 27 | CF | 6 | ASP | 9.9 |
| 28 | CG | 80 | THR | 9.9 |
| 22 | CA | 281 | C | 9.9 |
| 30 | CJ | 66 | SER | 9.9 |
| 55 | DI | 118 | ILE | 9.9 |
| 41 | CU | 47 | VAL | 9.9 |
| 14 | BN | 24 | ARG | 9.9 |
| 2 | BB | 16 | PHE | 9.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 52 | C5 | 21 | GLY | 9.9 |
| 2 | AB | 60 | ILE | 9.9 |
| 33 | CM | 114 | GLY | 9.9 |
| 30 | DJ | 95 | LYS | 9.8 |
| 44 | CX | 22 | GLY | 9.8 |
| 2 | AB | 111 | ILE | 9.8 |
| 39 | CS | 63 | VAL | 9.8 |
| 55 | DI | 35 | VAL | 9.8 |
| 30 | DJ | 27 | ALA | 9.8 |
| 30 | CJ | 121 | ASP | 9.8 |
| 45 | CY | 20 | HIS | 9.8 |
| 29 | DH | 81 | ALA | 9.8 |
| 13 | BM | 17 | ILE | 9.8 |
| 41 | CU | 43 | ILE | 9.8 |
| 30 | DJ | 19 | ASN | 9.8 |
| 28 | CG | 45 | HIS | 9.8 |
| 41 | CU | 51 | PHE | 9.8 |
| 9 | BI | 75 | GLN | 9.8 |
| 13 | BM | 48 | LEU | 9.8 |
| 28 | CG | 58 | TYR | 9.8 |
| 9 | BI | 127 | PHE | 9.8 |
| 30 | CJ | 84 | ALA | 9.7 |
| 12 | BL | 15 | LYS | 9.7 |
| 13 | BM | 58 | ASP | 9.7 |
| 28 | CG | 128 | GLN | 9.7 |
| 7 | BG | 112 | GLY | 9.7 |
| 22 | CA | 1870 | C | 9.7 |
| 3 | BC | 37 | PHE | 9.7 |
| 27 | CF | 157 | THR | 9.7 |
| 48 | C1 | 54 | VAL | 9.7 |
| 13 | BM | 94 | GLY | 9.7 |
| 30 | DJ | 141 | GLU | 9.7 |
| 55 | DI | 105 | LYS | 9.7 |
| 19 | AS | 5 | LEU | 9.7 |
| 42 | CV | 73 | PHE | 9.7 |
| 9 | BI | 68 | LYS | 9.7 |
| 30 | CJ | 95 | LYS | 9.7 |
| 25 | CD | 185 | ASN | 9.7 |
| 28 | CG | 76 | VAL | 9.7 |
| 30 | CJ | 24 | VAL | 9.7 |
| 30 | DJ | 43 | ASN | 9.7 |
| 13 | BM | 71 | ARG | 9.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 28 | CG | 82 | GLY | 9.6 |
| 55 | DI | 126 | LEU | 9.6 |
| 19 | BS | 3 | ARG | 9.6 |
| 30 | DJ | 92 | LYS | 9.6 |
| 30 | CJ | 113 | LYS | 9.6 |
| 13 | BM | 93 | ARG | 9.6 |
| 17 | BQ | 82 | ALA | 9.6 |
| 28 | CG | 78 | GLY | 9.6 |
| 30 | DJ | 37 | GLU | 9.6 |
| 13 | BM | 9 | ILE | 9.6 |
| 26 | CE | 8 | ALA | 9.6 |
| 53 | DA | 1172 | C | 9.6 |
| 27 | CF | 86 | GLY | 9.6 |
| 28 | CG | 156 | PRO | 9.6 |
| 7 | BG | 145 | ALA | 9.6 |
| 12 | BL | 124 | ALA | 9.6 |
| 13 | BM | 43 | VAL | 9.6 |
| 27 | CF | 108 | VAL | 9.6 |
| 13 | BM | 68 | ASP | 9.6 |
| 14 | BN | 4 | GLN | 9.6 |
| 13 | BM | 74 | SER | 9.6 |
| 27 | CF | 43 | ALA | 9.6 |
| 30 | CJ | 79 | LEU | 9.6 |
| 20 | BT | 80 | THR | 9.5 |
| 29 | DH | 146 | VAL | 9.5 |
| 13 | BM | 29 | ARG | 9.5 |
| 27 | CF | 138 | PHE | 9.5 |
| 41 | CU | 73 | ARG | 9.5 |
| 10 | BJ | 8 | ILE | 9.5 |
| 2 | BB | 226 | SER | 9.5 |
| 46 | CZ | 5 | GLU | 9.5 |
| 10 | BJ | 36 | VAL | 9.5 |
| 30 | CJ | 50 | GLU | 9.5 |
| 30 | CJ | 112 | THR | 9.5 |
| 46 | CZ | 30 | MET | 9.4 |
| 19 | BS | 18 | LYS | 9.4 |
| 30 | DJ | 12 | GLN | 9.4 |
| 55 | DI | 50 | VAL | 9.4 |
| 42 | CV | 21 | LYS | 9.4 |
| 13 | BM | 90 | ARG | 9.4 |
| 10 | BJ | 38 | GLY | 9.4 |
| 36 | CP | 110 | ALA | 9.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 40 | CT | 37 | THR | 9.4 |
| 1 | BA | 1024 | G | 9.4 |
| 7 | AG | 5 | ARG | 9.4 |
| 30 | DJ | 78 | VAL | 9.4 |
| 35 | CO | 119 | SER | 9.4 |
| 46 | CZ | 60 | LYS | 9.4 |
| 16 | AP | 45 | GLU | 9.4 |
| 10 | BJ | 28 | THR | 9.4 |
| 9 | BI | 39 | PHE | 9.3 |
| 46 | CZ | 22 | LEU | 9.3 |
| 1 | BA | 82 | G | 9.3 |
| 30 | CJ | 94 | ASN | 9.3 |
| 30 | CJ | 83 | ALA | 9.3 |
| 27 | CF | 31 | VAL | 9.3 |
| 27 | CF | 142 | ASP | 9.3 |
| 19 | BS | 24 | GLU | 9.3 |
| 42 | CV | 38 | GLY | 9.3 |
| 55 | DI | 21 | GLY | 9.3 |
| 28 | CG | 77 | ILE | 9.3 |
| 30 | CJ | 129 | ILE | 9.3 |
| 28 | CG | 9 | VAL | 9.3 |
| 36 | CP | 54 | VAL | 9.3 |
| 30 | DJ | 21 | SER | 9.3 |
| 14 | BN | 29 | ALA | 9.3 |
| 27 | CF | 135 | GLN | 9.3 |
| 42 | CV | 80 | ALA | 9.3 |
| 47 | C0 | 2 | ALA | 9.3 |
| 19 | BS | 64 | ASP | 9.3 |
| 2 | AB | 225 | ARG | 9.3 |
| 46 | CZ | 15 | ASN | 9.3 |
| 2 | BB | 219 | ALA | 9.3 |
| 6 | BF | 54 | LEU | 9.3 |
| 7 | BG | 118 | LEU | 9.3 |
| 22 | CA | 2121 | G | 9.3 |
| 55 | DI | 119 | PRO | 9.3 |
| 27 | CF | 77 | PHE | 9.2 |
| 10 | BJ | 76 | ILE | 9.2 |
| 28 | CG | 68 | ALA | 9.2 |
| 19 | BS | 57 | HIS | 9.2 |
| 26 | CE | 118 | LEU | 9.2 |
| 2 | BB | 139 | ARG | 9.2 |
| 29 | CH | 105 | ALA | 9.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 10 | BJ | 90 | LEU | 9.2 |
| 19 | BS | 47 | LEU | 9.2 |
| 42 | CV | 43 | LYS | 9.2 |
| 1 | BA | 1030 | U | 9.2 |
| 42 | CV | 71 | ALA | 9.2 |
| 3 | BC | 192 | THR | 9.2 |
| 7 | BG | 84 | THR | 9.2 |
| 16 | BP | 80 | LYS | 9.2 |
| 29 | DH | 65 | ALA | 9.2 |
| 41 | CU | 6 | ARG | 9.2 |
| 26 | CE | 104 | ALA | 9.1 |
| 36 | CP | 61 | GLN | 9.1 |
| 19 | BS | 17 | LYS | 9.1 |
| 26 | CE | 143 | LEU | 9.1 |
| 35 | CO | 63 | ARG | 9.1 |
| 9 | BI | 57 | MET | 9.1 |
| 7 | BG | 102 | ARG | 9.1 |
| 39 | CS | 49 | ILE | 9.1 |
| 55 | DI | 94 | ARG | 9.1 |
| 14 | BN | 51 | LEU | 9.1 |
| 10 | BJ | 74 | VAL | 9.1 |
| 29 | DH | 76 | GLU | 9.1 |
| 26 | CE | 19 | PHE | 9.1 |
| 30 | CJ | 46 | THR | 9.1 |
| 28 | CG | 112 | PRO | 9.1 |
| 29 | DH | 105 | ALA | 9.0 |
| 30 | CJ | 124 | ALA | 9.0 |
| 9 | AI | 90 | TYR | 9.0 |
| 41 | CU | 67 | VAL | 9.0 |
| 13 | BM | 82 | ASP | 9.0 |
| 53 | DA | 2165 | C | 9.0 |
| 13 | BM | 12 | HIS | 9.0 |
| 13 | BM | 69 | LEU | 9.0 |
| 30 | CJ | 115 | ALA | 9.0 |
| 22 | CA | 1107 | G | 9.0 |
| 7 | BG | 135 | VAL | 9.0 |
| 10 | BJ | 91 | ASP | 9.0 |
| 36 | CP | 49 | VAL | 9.0 |
| 28 | CG | 51 | THR | 9.0 |
| 30 | DJ | 65 | ARG | 9.0 |
| 30 | CJ | 85 | GLY | 9.0 |
| 36 | CP | 78 | VAL | 9.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 41 | CU | 57 | VAL | 9.0 |
| 51 | C4 | 52 | LYS | 9.0 |
| 27 | CF | 25 | VAL | 9.0 |
| 30 | DJ | 132 | THR | 9.0 |
| 42 | CV | 77 | THR | 9.0 |
| 27 | CF | 122 | PHE | 9.0 |
| 19 | BS | 45 | ILE | 9.0 |
| 37 | CQ | 4 | ILE | 9.0 |
| 7 | BG | 131 | LYS | 8.9 |
| 10 | BJ | 88 | MET | 8.9 |
| 30 | DJ | 121 | ASP | 8.9 |
| 2 | BB | 30 | PHE | 8.9 |
| 13 | BM | 86 | TYR | 8.9 |
| 55 | DI | 101 | LYS | 8.9 |
| 9 | BI | 42 | GLU | 8.9 |
| 41 | CU | 89 | GLU | 8.9 |
| 10 | BJ | 17 | LEU | 8.9 |
| 27 | CF | 50 | LEU | 8.9 |
| 10 | BJ | 97 | ASP | 8.9 |
| 14 | BN | 15 | ALA | 8.9 |
| 27 | CF | 119 | ALA | 8.9 |
| 28 | CG | 17 | VAL | 8.9 |
| 29 | CH | 47 | PHE | 8.9 |
| 38 | CR | 101 | PHE | 8.9 |
| 30 | CJ | 86 | ILE | 8.9 |
| 22 | CA | 1095 | A | 8.9 |
| 9 | BI | 118 | LEU | 8.9 |
| 13 | BM | 79 | ARG | 8.9 |
| 10 | BJ | 34 | ALA | 8.9 |
| 1 | AA | 86 | G | 8.9 |
| 2 | BB | 31 | ILE | 8.8 |
| 20 | BT | 9 | LYS | 8.8 |
| 36 | CP | 60 | GLU | 8.8 |
| 2 | BB | 12 | ALA | 8.8 |
| 55 | DI | 100 | ALA | 8.8 |
| 22 | CA | 1087 | G | 8.8 |
| 30 | DJ | 24 | VAL | 8.8 |
| 26 | CE | 136 | GLN | 8.8 |
| 36 | CP | 62 | LEU | 8.8 |
| 34 | CN | 21 | ALA | 8.8 |
| 1 | BA | 1033 | G | 8.8 |
| 29 | DH | 44 | ILE | 8.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 13 | BM | 34 | LEU | 8.8 |
| 31 | CK | 97 | PRO | 8.8 |
| 35 | CO | 100 | CYS | 8.8 |
| 42 | CV | 41 | LEU | 8.8 |
| 13 | AM | 114 | LYS | 8.8 |
| 22 | CA | 2184 | A | 8.7 |
| 29 | DH | 138 | VAL | 8.7 |
| 30 | DJ | 91 | GLY | 8.7 |
| 13 | BM | 25 | VAL | 8.7 |
| 33 | CM | 73 | ILE | 8.7 |
| 7 | BG | 76 | LYS | 8.7 |
| 29 | DH | 77 | THR | 8.7 |
| 49 | C2 | 53 | LYS | 8.7 |
| 49 | C2 | 47 | VAL | 8.7 |
| 20 | BT | 77 | ALA | 8.7 |
| 30 | CJ | 18 | ALA | 8.7 |
| 22 | CA | 1094 | U | 8.7 |
| 1 | BA | 1361 | G | 8.6 |
| 22 | CA | 1171 | G | 8.6 |
| 2 | BB | 4 | VAL | 8.6 |
| 26 | CE | 11 | ALA | 8.6 |
| 2 | AB | 139 | ARG | 8.6 |
| 22 | CA | 885 | C | 8.6 |
| 14 | BN | 39 | GLU | 8.6 |
| 33 | CM | 85 | VAL | 8.6 |
| 33 | CM | 121 | THR | 8.6 |
| 27 | CF | 174 | ASP | 8.6 |
| 10 | BJ | 92 | LEU | 8.6 |
| 34 | CN | 41 | LEU | 8.6 |
| 53 | DA | 2146 | C | 8.6 |
| 9 | BI | 126 | GLN | 8.6 |
| 33 | CM | 81 | ASP | 8.6 |
| 36 | CP | 47 | VAL | 8.6 |
| 30 | DJ | 90 | SER | 8.6 |
| 46 | CZ | 40 | SER | 8.6 |
| 7 | BG | 86 | GLN | 8.6 |
| 22 | CA | 1460 | U | 8.6 |
| 19 | BS | 71 | LEU | 8.6 |
| 46 | CZ | 56 | LEU | 8.6 |
| 55 | DI | 47 | GLU | 8.6 |
| 36 | CP | 71 | ALA | 8.6 |
| 9 | BI | 66 | THR | 8.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 30 | CJ | 78 | VAL | 8.6 |
| 13 | BM | 8 | ASN | 8.6 |
| 28 | CG | 105 | LEU | 8.5 |
| 42 | CV | 6 | ARG | 8.5 |
| 44 | CX | 33 | ALA | 8.5 |
| 36 | CP | 82 | ALA | 8.5 |
| 30 | DJ | 46 | THR | 8.5 |
| 1 | BA | 1534 | A | 8.5 |
| 25 | CD | 8 | LYS | 8.5 |
| 33 | CM | 124 | GLY | 8.5 |
| 9 | BI | 44 | ALA | 8.5 |
| 33 | CM | 108 | ALA | 8.5 |
| 17 | BQ | 74 | THR | 8.5 |
| 2 | BB | 57 | LEU | 8.5 |
| 3 | BC | 122 | SER | 8.5 |
| 25 | CD | 14 | ILE | 8.5 |
| 25 | CD | 96 | ILE | 8.5 |
| 28 | CG | 132 | VAL | 8.5 |
| 32 | CL | 88 | ASN | 8.5 |
| 42 | CV | 59 | VAL | 8.5 |
| 27 | CF | 96 | MET | 8.5 |
| 2 | BB | 117 | LEU | 8.5 |
| 14 | AN | 51 | LEU | 8.5 |
| 10 | BJ | 40 | ILE | 8.5 |
| 30 | CJ | 82 | LYS | 8.5 |
| 46 | CZ | 58 | ASN | 8.4 |
| 7 | BG | 57 | SER | 8.4 |
| 22 | CA | 2120 | G | 8.4 |
| 27 | CF | 11 | GLU | 8.4 |
| 29 | DH | 147 | VAL | 8.4 |
| 46 | DZ | 63 | ALA | 8.4 |
| 7 | BG | 78 | ARG | 8.4 |
| 32 | CL | 89 | ASN | 8.4 |
| 1 | BA | 1244 | G | 8.4 |
| 9 | BI | 26 | GLY | 8.4 |
| 41 | CU | 72 | GLN | 8.4 |
| 29 | DH | 137 | GLU | 8.4 |
| 10 | BJ | 101 | SER | 8.4 |
| 27 | CF | 99 | PHE | 8.4 |
| 30 | CJ | 55 | ILE | 8.4 |
| 55 | DI | 38 | MET | 8.4 |
| 29 | CH | 140 | ALA | 8.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 53 | DA | 2166 | U | 8.4 |
| 10 | BJ | 102 | LEU | 8.4 |
| 19 | BS | 16 | LEU | 8.4 |
| 53 | DA | 2114 | A | 8.4 |
| 22 | CA | 228 | C | 8.3 |
| 14 | BN | 40 | ASP | 8.3 |
| 29 | CH | 3 | VAL | 8.3 |
| 30 | CJ | 88 | SER | 8.3 |
| 14 | BN | 53 | ARG | 8.3 |
| 20 | BT | 51 | PHE | 8.3 |
| 51 | C4 | 22 | PHE | 8.3 |
| 22 | CA | 878 | A | 8.3 |
| 26 | CE | 173 | THR | 8.3 |
| 19 | BS | 80 | TYR | 8.3 |
| 55 | DI | 64 | VAL | 8.3 |
| 22 | CA | 2169 | A | 8.3 |
| 42 | CV | 74 | ASN | 8.3 |
| 7 | BG | 104 | ILE | 8.3 |
| 27 | CF | 137 | ILE | 8.3 |
| 28 | CG | 121 | ILE | 8.3 |
| 30 | DJ | 15 | ALA | 8.3 |
| 20 | BT | 49 | LYS | 8.3 |
| 30 | CJ | 100 | LYS | 8.3 |
| 30 | CJ | 89 | GLY | 8.3 |
| 7 | BG | 94 | VAL | 8.3 |
| 27 | CF | 27 | GLN | 8.2 |
| 55 | DI | 27 | VAL | 8.2 |
| 27 | CF | 91 | LEU | 8.2 |
| 36 | CP | 12 | THR | 8.2 |
| 36 | CP | 50 | ALA | 8.2 |
| 27 | CF | 85 | ILE | 8.2 |
| 37 | CQ | 43 | PHE | 8.2 |
| 26 | CE | 138 | LEU | 8.2 |
| 30 | DJ | 124 | ALA | 8.2 |
| 33 | CM | 142 | ILE | 8.2 |
| 38 | CR | 15 | LYS | 8.2 |
| 36 | CP | 64 | TYR | 8.2 |
| 3 | BC | 146 | ALA | 8.2 |
| 10 | BJ | 21 | ALA | 8.2 |
| 1 | BA | 1019 | A | 8.2 |
| 19 | BS | 31 | LEU | 8.2 |
| 42 | CV | 60 | GLU | 8.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | BF | 70 | VAL | 8.2 |
| 26 | CE | 14 | VAL | 8.2 |
| 46 | CZ | 37 | LEU | 8.2 |
| 55 | DI | 71 | CYS | 8.2 |
| 1 | BA | 1025 | U | 8.2 |
| 22 | CA | 2170 | A | 8.2 |
| 17 | BQ | 70 | THR | 8.2 |
| 2 | AB | 7 | ARG | 8.2 |
| 26 | CE | 3 | LEU | 8.2 |
| 42 | CV | 98 | SER | 8.1 |
| 10 | BJ | 93 | ALA | 8.1 |
| 36 | CP | 20 | GLU | 8.1 |
| 3 | BC | 138 | VAL | 8.1 |
| 29 | CH | 108 | VAL | 8.1 |
| 48 | C1 | 3 | VAL | 8.1 |
| 2 | AB | 57 | LEU | 8.1 |
| 29 | CH | 17 | ASP | 8.1 |
| 22 | CA | 1092 | C | 8.1 |
| 1 | BA | 1013 | G | 8.1 |
| 13 | AM | 4 | ILE | 8.1 |
| 29 | CH | 142 | VAL | 8.1 |
| 53 | DA | 1175 | A | 8.1 |
| 28 | CG | 69 | ARG | 8.1 |
| 13 | AM | 9 | ILE | 8.1 |
| 19 | BS | 50 | ALA | 8.1 |
| 28 | CG | 131 | ILE | 8.1 |
| 2 | BB | 123 | ASP | 8.1 |
| 2 | BB | 210 | VAL | 8.1 |
| 13 | BM | 60 | VAL | 8.1 |
| 55 | DI | 76 | PHE | 8.1 |
| 51 | C4 | 20 | GLY | 8.1 |
| 7 | BG | 124 | LEU | 8.1 |
| 30 | DJ | 134 | ARG | 8.1 |
| 14 | AN | 30 | ILE | 8.1 |
| 30 | CJ | 39 | CYS | 8.1 |
| 19 | BS | 21 | LYS | 8.0 |
| 30 | DJ | 97 | LYS | 8.0 |
| 53 | DA | 2120 | G | 8.0 |
| 41 | CU | 46 | ALA | 8.0 |
| 2 | BB | 217 | VAL | 8.0 |
| 34 | CN | 131 | VAL | 8.0 |
| 43 | CW | 92 | VAL | 8.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 20 | BT | 46 | ALA | 8.0 |
| 13 | AM | 3 | ARG | 8.0 |
| 27 | CF | 118 | SER | 8.0 |
| 2 | BB | 80 | VAL | 8.0 |
| 9 | BI | 54 | LEU | 8.0 |
| 27 | CF | 16 | LEU | 8.0 |
| 40 | CT | 110 | ARG | 8.0 |
| 19 | BS | 41 | PHE | 8.0 |
| 22 | CA | 2128 | G | 8.0 |
| 27 | CF | 66 | LEU | 8.0 |
| 29 | CH | 144 | VAL | 8.0 |
| 26 | CE | 1 | MET | 8.0 |
| 53 | DA | 654 | A | 8.0 |
| 25 | CD | 86 | GLU | 8.0 |
| 9 | BI | 21 | ILE | 8.0 |
| 55 | DI | 66 | GLY | 7.9 |
| 20 | BT | 85 | LYS | 7.9 |
| 29 | DH | 124 | THR | 7.9 |
| 35 | CO | 28 | LEU | 7.9 |
| 29 | CH | 107 | GLY | 7.9 |
| 22 | CA | 2106 | U | 7.9 |
| 30 | CJ | 53 | LEU | 7.9 |
| 43 | CW | 34 | LYS | 7.9 |
| 30 | CJ | 128 | SER | 7.9 |
| 30 | CJ | 126 | THR | 7.9 |
| 30 | CJ | 136 | MET | 7.9 |
| 29 | DH | 143 | ILE | 7.9 |
| 55 | DI | 120 | ALA | 7.9 |
| 2 | AB | 135 | LEU | 7.9 |
| 13 | AM | 48 | LEU | 7.9 |
| 13 | BM | 19 | LEU | 7.9 |
| 22 | CA | 2168 | G | 7.9 |
| 33 | CM | 15 | ALA | 7.9 |
| 29 | DH | 107 | GLY | 7.9 |
| 39 | CS | 37 | GLU | 7.9 |
| 53 | DA | 2175 | C | 7.9 |
| 7 | BG | 25 | LYS | 7.8 |
| 32 | CL | 91 | SER | 7.8 |
| 22 | CA | 2119 | A | 7.8 |
| 40 | CT | 66 | ILE | 7.8 |
| 40 | CT | 36 | LEU | 7.8 |
| 27 | CF | 51 | ASP | 7.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 39 | CS | 43 | ASN | 7.8 |
| 31 | CK | 55 | ILE | 7.8 |
| 1 | BA | 1138 | G | 7.8 |
| 41 | CU | 70 | HIS | 7.8 |
| 27 | CF | 56 | ASP | 7.8 |
| 3 | BC | 145 | GLY | 7.8 |
| 27 | CF | 92 | ARG | 7.8 |
| 28 | CG | 107 | LEU | 7.8 |
| 39 | CS | 32 | THR | 7.8 |
| 16 | BP | 45 | GLU | 7.8 |
| 27 | CF | 2 | ALA | 7.8 |
| 9 | BI | 129 | LYS | 7.8 |
| 13 | BM | 11 | ASP | 7.8 |
| 27 | CF | 129 | SER | 7.8 |
| 29 | CH | 136 | SER | 7.8 |
| 41 | CU | 2 | ILE | 7.8 |
| 55 | DI | 91 | ALA | 7.8 |
| 7 | AG | 20 | SER | 7.8 |
| 25 | CD | 25 | THR | 7.8 |
| 28 | CG | 171 | THR | 7.8 |
| 29 | CH | 20 | ASN | 7.8 |
| 30 | CJ | 92 | LYS | 7.8 |
| 21 | AU | 3 | VAL | 7.8 |
| 26 | CE | 28 | VAL | 7.8 |
| 22 | CA | 2178 | C | 7.7 |
| 22 | CA | 1084 | A | 7.7 |
| 26 | CE | 134 | LEU | 7.7 |
| 55 | DI | 82 | ILE | 7.7 |
| 36 | CP | 80 | GLU | 7.7 |
| 2 | BB | 63 | ARG | 7.7 |
| 22 | CA | 1053 | C | 7.7 |
| 29 | CH | 74 | ALA | 7.7 |
| 27 | CF | 132 | VAL | 7.7 |
| 41 | CU | 16 | VAL | 7.7 |
| 30 | CJ | 131 | GLY | 7.7 |
| 27 | CF | 102 | ARG | 7.7 |
| 26 | CE | 189 | THR | 7.7 |
| 1 | BA | 1243 | C | 7.7 |
| 28 | CG | 101 | ASN | 7.7 |
| 55 | DI | 92 | ALA | 7.7 |
| 10 | BJ | 98 | VAL | 7.7 |
| 28 | CG | 79 | VAL | 7.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 20 | BT | 34 | LYS | 7.7 |
| 22 | CA | 2112 | G | 7.7 |
| 44 | CX | 83 | GLU | 7.7 |
| 42 | CV | 27 | ASN | 7.7 |
| 30 | CJ | 133 | ALA | 7.7 |
| 26 | CE | 77 | ILE | 7.7 |
| 26 | CE | 175 | ILE | 7.7 |
| 27 | CF | 15 | LYS | 7.7 |
| 10 | BJ | 96 | VAL | 7.7 |
| 22 | CA | 316 | C | 7.7 |
| 7 | BG | 148 | ASN | 7.7 |
| 2 | BB | 11 | LYS | 7.7 |
| 36 | CP | 41 | ALA | 7.7 |
| 29 | CH | 12 | LEU | 7.6 |
| 42 | CV | 48 | PRO | 7.6 |
| 14 | BN | 73 | PHE | 7.6 |
| 21 | AU | 12 | PHE | 7.6 |
| 44 | CX | 46 | HIS | 7.6 |
| 27 | CF | 33 | LYS | 7.6 |
| 46 | CZ | 4 | LYS | 7.6 |
| 14 | BN | 55 | SER | 7.6 |
| 7 | BG | 81 | GLY | 7.6 |
| 55 | DI | 75 | ALA | 7.6 |
| 1 | BA | 85 | U | 7.6 |
| 42 | CV | 33 | LYS | 7.6 |
| 22 | CA | 882 | G | 7.6 |
| 27 | CF | 153 | ASP | 7.6 |
| 41 | CU | 37 | ASP | 7.6 |
| 25 | CD | 95 | SER | 7.6 |
| 42 | CV | 17 | LYS | 7.6 |
| 7 | AG | 49 | THR | 7.6 |
| 29 | DH | 61 | VAL | 7.6 |
| 44 | CX | 79 | PHE | 7.6 |
| 43 | CW | 67 | GLY | 7.6 |
| 16 | AP | 81 | ALA | 7.6 |
| 30 | CJ | 104 | ALA | 7.6 |
| 30 | DJ | 8 | TYR | 7.6 |
| 30 | CJ | 77 | ALA | 7.6 |
| 19 | AS | 41 | PHE | 7.6 |
| 30 | CJ | 54 | PRO | 7.6 |
| 27 | CF | 164 | GLU | 7.6 |
| 30 | DJ | 50 | GLU | 7.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | AA | 1026 | G | 7.5 |
| 13 | BM | 24 | GLY | 7.5 |
| 22 | CA | 1071 | G | 7.5 |
| 28 | CG | 25 | THR | 7.5 |
| 30 | CJ | 45 | LYS | 7.5 |
| 10 | BJ | 27 | GLU | 7.5 |
| 22 | CA | 2125 | G | 7.5 |
| 53 | DA | 2115 | G | 7.5 |
| 30 | CJ | 49 | ILE | 7.5 |
| 36 | CP | 67 | ASN | 7.5 |
| 42 | CV | 85 | PHE | 7.5 |
| 55 | DI | 45 | GLY | 7.5 |
| 22 | CA | 1172 | C | 7.5 |
| 2 | AB | 49 | MET | 7.5 |
| 7 | BG | 43 | VAL | 7.5 |
| 34 | CN | 22 | GLN | 7.5 |
| 1 | BA | 1304 | G | 7.5 |
| 27 | CF | 14 | LYS | 7.5 |
| 19 | BS | 37 | ARG | 7.5 |
| 16 | AP | 47 | GLU | 7.5 |
| 25 | CD | 73 | VAL | 7.5 |
| 14 | AN | 46 | LEU | 7.4 |
| 7 | BG | 107 | ALA | 7.4 |
| 28 | CG | 59 | ALA | 7.4 |
| 40 | CT | 68 | ASP | 7.4 |
| 33 | CM | 93 | ASN | 7.4 |
| 2 | BB | 126 | PHE | 7.4 |
| 7 | AG | 48 | GLU | 7.4 |
| 7 | BG | 109 | ARG | 7.4 |
| 13 | BM | 101 | ARG | 7.4 |
| 28 | CG | 106 | SER | 7.4 |
| 25 | CD | 92 | VAL | 7.4 |
| 41 | DU | 1 | MET | 7.4 |
| 34 | CN | 60 | GLN | 7.4 |
| 30 | DJ | 126 | THR | 7.4 |
| 30 | CJ | 137 | GLY | 7.4 |
| 30 | DJ | 128 | SER | 7.4 |
| 2 | AB | 14 | VAL | 7.4 |
| 14 | BN | 14 | VAL | 7.4 |
| 26 | CE | 165 | HIS | 7.4 |
| 1 | AA | 82 | G | 7.4 |
| 1 | BA | 1022 | A | 7.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 14 | BN | 75 | ARG | 7.4 |
| 41 | CU | 34 | VAL | 7.4 |
| 7 | BG | 18 | PHE | 7.4 |
| 22 | CA | 318 | C | 7.4 |
| 26 | CE | 153 | LEU | 7.4 |
| 36 | CP | 116 | GLN | 7.4 |
| 30 | CJ | 40 | LYS | 7.3 |
| 30 | DJ | 59 | ILE | 7.3 |
| 22 | CA | 1170 | C | 7.3 |
| 3 | BC | 53 | SER | 7.3 |
| 7 | BG | 20 | SER | 7.3 |
| 53 | DA | 2105 | U | 7.3 |
| 1 | BA | 207 | C | 7.3 |
| 19 | BS | 19 | VAL | 7.3 |
| 33 | CM | 122 | VAL | 7.3 |
| 9 | BI | 110 | GLN | 7.3 |
| 14 | BN | 16 | LEU | 7.3 |
| 42 | DV | 52 | LEU | 7.3 |
| 36 | CP | 63 | LYS | 7.3 |
| 1 | BA | 1362 | A | 7.3 |
| 39 | CS | 38 | VAL | 7.3 |
| 22 | CA | 2104 | C | 7.3 |
| 22 | CA | 1059 | G | 7.3 |
| 11 | BK | 16 | VAL | 7.3 |
| 30 | DJ | 105 | GLN | 7.3 |
| 41 | CU | 68 | LYS | 7.3 |
| 27 | CF | 90 | THR | 7.3 |
| 2 | AB | 6 | MET | 7.3 |
| 25 | CD | 10 | GLY | 7.2 |
| 3 | BC | 107 | ARG | 7.2 |
| 9 | AI | 129 | LYS | 7.2 |
| 27 | CF | 20 | PHE | 7.2 |
| 29 | CH | 135 | HIS | 7.2 |
| 33 | CM | 61 | LEU | 7.2 |
| 2 | AB | 12 | ALA | 7.2 |
| 21 | AU | 53 | VAL | 7.2 |
| 29 | CH | 145 | ASN | 7.2 |
| 30 | DJ | 123 | GLU | 7.2 |
| 32 | CL | 35 | VAL | 7.2 |
| 27 | CF | 162 | SER | 7.2 |
| 42 | CV | 96 | PHE | 7.2 |
| 32 | CL | 110 | GLU | 7.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 10 | AJ | 26 | VAL | 7.2 |
| 9 | BI | 14 | SER | 7.2 |
| 7 | BG | 58 | GLU | 7.2 |
| 26 | CE | 122 | GLU | 7.2 |
| 30 | DJ | 113 | LYS | 7.2 |
| 7 | BG | 111 | ARG | 7.2 |
| 44 | CX | 47 | ALA | 7.2 |
| 48 | C1 | 44 | THR | 7.2 |
| 55 | DI | 67 | THR | 7.2 |
| 31 | CK | 127 | GLY | 7.2 |
| 37 | CQ | 92 | VAL | 7.2 |
| 40 | CT | 107 | VAL | 7.2 |
| 2 | AB | 42 | ASN | 7.2 |
| 34 | CN | 59 | ARG | 7.2 |
| 53 | DA | 2174 | C | 7.2 |
| 14 | AN | 36 | ALA | 7.2 |
| 26 | CE | 199 | MET | 7.2 |
| 28 | CG | 125 | CYS | 7.2 |
| 29 | DH | 142 | VAL | 7.2 |
| 24 | CC | 64 | ILE | 7.2 |
| 26 | CE | 149 | ILE | 7.2 |
| 33 | CM | 100 | ILE | 7.2 |
| 53 | DA | 1077 | A | 7.2 |
| 53 | DA | 2101 | A | 7.2 |
| 29 | DH | 127 | GLU | 7.2 |
| 28 | CG | 148 | LEU | 7.1 |
| 9 | BI | 119 | ARG | 7.1 |
| 44 | CX | 50 | ASN | 7.1 |
| 3 | AC | 82 | GLU | 7.1 |
| 3 | BC | 181 | ASP | 7.1 |
| 39 | CS | 88 | GLY | 7.1 |
| 36 | CP | 51 | ALA | 7.1 |
| 31 | CK | 128 | ASN | 7.1 |
| 39 | CS | 52 | PRO | 7.1 |
| 2 | BB | 33 | GLY | 7.1 |
| 42 | CV | 101 | GLU | 7.1 |
| 52 | C5 | 6 | SER | 7.1 |
| 22 | CA | 41 | C | 7.1 |
| 55 | DI | 72 | LEU | 7.1 |
| 3 | BC | 62 | LYS | 7.1 |
| 19 | AS | 11 | ILE | 7.1 |
| 1 | AA | 79 | G | 7.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 22 | CA | 654 | A | 7.1 |
| 27 | CF | 177 | PHE | 7.1 |
| 9 | AI | 53 | GLU | 7.1 |
| 35 | CO | 62 | ASN | 7.1 |
| 1 | BA | 210 | C | 7.1 |
| 1 | BA | 1245 | C | 7.1 |
| 31 | CK | 137 | PRO | 7.1 |
| 13 | AM | 36 | ALA | 7.1 |
| 29 | DH | 125 | THR | 7.1 |
| 22 | CA | 317 | G | 7.1 |
| 42 | CV | 5 | ILE | 7.1 |
| 33 | CM | 19 | LEU | 7.1 |
| 10 | BJ | 75 | ASP | 7.1 |
| 17 | BQ | 50 | ASN | 7.1 |
| 29 | CH | 16 | GLY | 7.1 |
| 15 | BO | 89 | ARG | 7.1 |
| 27 | CF | 81 | GLN | 7.1 |
| 30 | DJ | 81 | LYS | 7.1 |
| 41 | CU | 62 | VAL | 7.1 |
| 33 | CM | 83 | ALA | 7.0 |
| 36 | CP | 106 | LEU | 7.0 |
| 2 | BB | 74 | ARG | 7.0 |
| 26 | CE | 129 | PRO | 7.0 |
| 3 | BC | 56 | VAL | 7.0 |
| 29 | DH | 104 | THR | 7.0 |
| 3 | BC | 77 | ILE | 7.0 |
| 2 | BB | 69 | PHE | 7.0 |
| 10 | BJ | 45 | ARG | 7.0 |
| 22 | CA | 2158 | A | 7.0 |
| 29 | DH | 56 | ALA | 7.0 |
| 7 | BG | 105 | VAL | 7.0 |
| 29 | DH | 95 | GLY | 7.0 |
| 33 | CM | 78 | ARG | 7.0 |
| 10 | BJ | 67 | ILE | 7.0 |
| 29 | CH | 143 | ILE | 7.0 |
| 3 | BC | 98 | PRO | 7.0 |
| 10 | BJ | 85 | ASP | 7.0 |
| 1 | BA | 948 | C | 7.0 |
| 1 | BA | 1359 | C | 7.0 |
| 42 | CV | 19 | LYS | 7.0 |
| 9 | AI | 88 | MET | 7.0 |
| 17 | BQ | 17 | MET | 7.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 37 | CQ | 85 | SER | 7.0 |
| 30 | CJ | 37 | GLU | 7.0 |
| 39 | CS | 22 | LEU | 7.0 |
| 53 | DA | 2164 | C | 7.0 |
| 36 | CP | 25 | ARG | 7.0 |
| 42 | CV | 82 | ARG | 7.0 |
| 14 | BN | 17 | ALA | 7.0 |
| 5 | BE | 23 | LYS | 7.0 |
| 9 | BI | 6 | TYR | 7.0 |
| 9 | BI | 116 | VAL | 7.0 |
| 27 | DF | 83 | TYR | 7.0 |
| 35 | CO | 29 | VAL | 7.0 |
| 38 | CR | 39 | VAL | 7.0 |
| 21 | AU | 2 | PRO | 7.0 |
| 20 | BT | 3 | ASN | 7.0 |
| 2 | AB | 214 | LEU | 7.0 |
| 46 | CZ | 36 | GLN | 7.0 |
| 2 | AB | 90 | PHE | 7.0 |
| 40 | CT | 39 | THR | 7.0 |
| 1 | BA | 1006 | G | 7.0 |
| 27 | CF | 48 | LYS | 7.0 |
| 11 | BK | 55 | SER | 7.0 |
| 28 | CG | 46 | ALA | 7.0 |
| 36 | CP | 76 | LYS | 6.9 |
| 33 | CM | 3 | LEU | 6.9 |
| 39 | CS | 59 | ILE | 6.9 |
| 7 | BG | 144 | MET | 6.9 |
| 41 | CU | 60 | THR | 6.9 |
| 1 | BA | 204 | G | 6.9 |
| 27 | CF | 52 | ASN | 6.9 |
| 22 | CA | 1076 | C | 6.9 |
| 22 | CA | 1868 | C | 6.9 |
| 32 | CL | 112 | PHE | 6.9 |
| 33 | CM | 107 | PHE | 6.9 |
| 10 | AJ | 93 | ALA | 6.9 |
| 52 | C5 | 33 | HIS | 6.9 |
| 17 | AQ | 83 | VAL | 6.9 |
| 39 | CS | 20 | VAL | 6.9 |
| 1 | AA | 78 | A | 6.9 |
| 27 | CF | 17 | MET | 6.9 |
| 17 | BQ | 61 | ILE | 6.9 |
| 20 | BT | 86 | LEU | 6.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 36 | CP | 56 | LYS | 6.9 |
| 46 | CZ | 21 | LEU | 6.9 |
| 27 | CF | 175 | PHE | 6.9 |
| 30 | DJ | 108 | GLU | 6.9 |
| 46 | CZ | 59 | GLU | 6.9 |
| 26 | CE | 140 | ASP | 6.9 |
| 7 | BG | 6 | VAL | 6.9 |
| 28 | CG | 86 | LYS | 6.9 |
| 2 | AB | 58 | ASN | 6.9 |
| 26 | CE | 133 | LEU | 6.9 |
| 53 | DA | 2111 | U | 6.9 |
| 30 | DJ | 31 | GLN | 6.9 |
| 13 | BM | 99 | GLY | 6.9 |
| 22 | CA | 549 | G | 6.9 |
| 36 | CP | 111 | ARG | 6.9 |
| 26 | CE | 98 | LYS | 6.9 |
| 46 | CZ | 32 | ALA | 6.9 |
| 22 | CA | 2177 | C | 6.9 |
| 10 | BJ | 95 | GLY | 6.8 |
| 22 | CA | 1406 | U | 6.8 |
| 36 | CP | 75 | GLY | 6.8 |
| 26 | CE | 150 | THR | 6.8 |
| 33 | CM | 120 | VAL | 6.8 |
| 47 | C0 | 55 | VAL | 6.8 |
| 14 | BN | 49 | GLN | 6.8 |
| 22 | CA | 361 | G | 6.8 |
| 14 | AN | 39 | GLU | 6.8 |
| 55 | DI | 96 | PHE | 6.8 |
| 6 | BF | 79 | ARG | 6.8 |
| 18 | AR | 73 | ARG | 6.8 |
| 29 | DH | 135 | HIS | 6.8 |
| 43 | CW | 60 | VAL | 6.8 |
| 14 | BN | 2 | ALA | 6.8 |
| 55 | DI | 22 | ALA | 6.8 |
| 9 | BI | 34 | SER | 6.8 |
| 42 | CV | 58 | ILE | 6.8 |
| 10 | BJ | 56 | HIS | 6.8 |
| 50 | C3 | 1 | MET | 6.8 |
| 22 | CA | 275 | C | 6.8 |
| 22 | CA | 2174 | C | 6.8 |
| 36 | CP | 53 | THR | 6.8 |
| 27 | CF | 110 | ARG | 6.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 14 | AN | 37 | SER | 6.8 |
| 14 | AN | 49 | GLN | 6.8 |
| 19 | BS | 44 | MET | 6.8 |
| 22 | CA | 896 | A | 6.8 |
| 40 | CT | 92 | ARG | 6.8 |
| 53 | DA | 283 | G | 6.8 |
| 2 | BB | 65 | GLY | 6.8 |
| 2 | BB | 206 | ALA | 6.8 |
| 14 | BN | 82 | ILE | 6.8 |
| 33 | CM | 4 | ASN | 6.8 |
| 22 | CA | 883 | G | 6.8 |
| 24 | CC | 27 | GLY | 6.8 |
| 43 | CW | 33 | GLY | 6.8 |
| 20 | BT | 50 | ALA | 6.8 |
| 35 | CO | 77 | ALA | 6.8 |
| 27 | CF | 149 | VAL | 6.8 |
| 29 | CH | 115 | VAL | 6.8 |
| 9 | AI | 54 | LEU | 6.7 |
| 48 | C1 | 39 | LEU | 6.7 |
| 10 | BJ | 6 | ILE | 6.7 |
| 27 | CF | 158 | THR | 6.7 |
| 28 | CG | 49 | THR | 6.7 |
| 26 | CE | 20 | GLY | 6.7 |
| 15 | BO | 15 | PHE | 6.7 |
| 40 | CT | 54 | ALA | 6.7 |
| 3 | BC | 102 | ASN | 6.7 |
| 27 | CF | 49 | LEU | 6.7 |
| 53 | DA | 2113 | U | 6.7 |
| 55 | DI | 97 | LYS | 6.7 |
| 1 | BA | 1325 | C | 6.7 |
| 2 | BB | 198 | PHE | 6.7 |
| 38 | CR | 71 | GLN | 6.7 |
| 9 | AI | 58 | VAL | 6.7 |
| 10 | BJ | 52 | LEU | 6.7 |
| 6 | AF | 97 | THR | 6.7 |
| 27 | CF | 141 | ILE | 6.7 |
| 53 | DA | 138 | U | 6.7 |
| 53 | DA | 2133 | G | 6.7 |
| 33 | CM | 137 | ALA | 6.7 |
| 36 | CP | 57 | ALA | 6.7 |
| 55 | DI | 73 | LYS | 6.7 |
| 41 | CU | 58 | VAL | 6.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | CJ | 48 | SER | 6.7 |
| 22 | CA | 879 | G | 6.7 |
| 22 | CA | 1169 | A | 6.7 |
| 13 | BM | 33 | ILE | 6.7 |
| 20 | BT | 24 | ARG | 6.7 |
| 33 | CM | 102 | GLY | 6.7 |
| 14 | BN | 19 | LYS | 6.7 |
| 19 | BS | 62 | VAL | 6.7 |
| 29 | CH | 9 | VAL | 6.7 |
| 53 | DA | 277 | G | 6.7 |
| 20 | BT | 41 | ALA | 6.7 |
| 25 | CD | 71 | ALA | 6.7 |
| 42 | CV | 24 | LYS | 6.7 |
| 19 | BS | 43 | ASN | 6.7 |
| 10 | BJ | 80 | THR | 6.6 |
| 22 | CA | 2180 | U | 6.6 |
| 29 | DH | 134 | VAL | 6.6 |
| 30 | DJ | 61 | VAL | 6.6 |
| 37 | CQ | 25 | THR | 6.6 |
| 53 | DA | 2132 | U | 6.6 |
| 2 | AB | 10 | LEU | 6.6 |
| 9 | BI | 7 | TYR | 6.6 |
| 14 | BN | 20 | TYR | 6.6 |
| 19 | BS | 56 | GLN | 6.6 |
| 3 | BC | 162 | ILE | 6.6 |
| 55 | DI | 107 | GLU | 6.6 |
| 7 | BG | 54 | SER | 6.6 |
| 30 | CJ | 135 | SER | 6.6 |
| 27 | CF | 18 | THR | 6.6 |
| 11 | BK | 65 | VAL | 6.6 |
| 26 | CE | 147 | LEU | 6.6 |
| 10 | BJ | 33 | GLY | 6.6 |
| 36 | CP | 70 | ALA | 6.6 |
| 2 | BB | 164 | ILE | 6.6 |
| 36 | CP | 29 | HIS | 6.6 |
| 28 | CG | 170 | ARG | 6.6 |
| 36 | CP | 105 | ALA | 6.6 |
| 41 | CU | 88 | LYS | 6.6 |
| 50 | C3 | 42 | LEU | 6.6 |
| 53 | DA | 2147 | A | 6.6 |
| 36 | CP | 99 | TYR | 6.6 |
| 1 | BA | 1247 | U | 6.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | BA | 79 | G | 6.6 |
| 22 | CA | 914 | G | 6.6 |
| 29 | DH | 108 | VAL | 6.6 |
| 30 | DJ | 20 | PRO | 6.6 |
| 37 | CQ | 17 | VAL | 6.6 |
| 42 | CV | 83 | VAL | 6.6 |
| 1 | BA | 983 | A | 6.6 |
| 19 | AS | 13 | LEU | 6.6 |
| 29 | DH | 52 | ALA | 6.6 |
| 43 | CW | 28 | ALA | 6.6 |
| 2 | AB | 31 | ILE | 6.6 |
| 3 | BC | 80 | LYS | 6.6 |
| 9 | BI | 43 | THR | 6.6 |
| 30 | DJ | 75 | PRO | 6.6 |
| 7 | AG | 80 | VAL | 6.6 |
| 41 | CU | 91 | GLN | 6.6 |
| 43 | CW | 22 | ALA | 6.6 |
| 3 | BC | 27 | LYS | 6.6 |
| 13 | BM | 44 | LYS | 6.6 |
| 36 | CP | 69 | ASP | 6.6 |
| 2 | BB | 225 | ARG | 6.6 |
| 42 | CV | 65 | ILE | 6.6 |
| 1 | AA | 1032 | G | 6.5 |
| 1 | BA | 1287 | A | 6.5 |
| 7 | BG | 151 | PHE | 6.5 |
| 53 | DA | 1171 | G | 6.5 |
| 36 | CP | 3 | LYS | 6.5 |
| 46 | CZ | 10 | SER | 6.5 |
| 26 | CE | 5 | LEU | 6.5 |
| 41 | CU | 87 | LEU | 6.5 |
| 29 | DH | 123 | ARG | 6.5 |
| 46 | CZ | 29 | ARG | 6.5 |
| 27 | CF | 47 | LYS | 6.5 |
| 27 | CF | 60 | ILE | 6.5 |
| 30 | CJ | 93 | PRO | 6.5 |
| 33 | CM | 80 | SER | 6.5 |
| 10 | BJ | 37 | ARG | 6.5 |
| 14 | BN | 38 | ASP | 6.5 |
| 28 | CG | 13 | ALA | 6.5 |
| 52 | C5 | 12 | ARG | 6.5 |
| 2 | AB | 114 | LEU | 6.5 |
| 7 | BG | 30 | LEU | 6.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 35 | CO | 9 | GLN | 6.5 |
| 22 | CA | 881 | G | 6.5 |
| 6 | BF | 66 | ALA | 6.5 |
| 26 | CE | 124 | PHE | 6.5 |
| 28 | CG | 65 | ALA | 6.5 |
| 18 | BR | 20 | GLU | 6.5 |
| 28 | CG | 41 | VAL | 6.5 |
| 32 | CL | 68 | GLY | 6.5 |
| 22 | CA | 1176 | U | 6.5 |
| 13 | BM | 81 | MET | 6.5 |
| 30 | CJ | 130 | GLU | 6.5 |
| 53 | DA | 2103 | C | 6.5 |
| 29 | CH | 120 | GLY | 6.5 |
| 55 | DI | 12 | VAL | 6.5 |
| 22 | CA | 2105 | U | 6.5 |
| 36 | CP | 83 | LEU | 6.5 |
| 22 | CA | 1179 | G | 6.5 |
| 1 | BA | 1027 | C | 6.5 |
| 26 | CE | 37 | ALA | 6.5 |
| 30 | DJ | 104 | ALA | 6.5 |
| 40 | CT | 5 | ALA | 6.5 |
| 53 | DA | 2135 | A | 6.5 |
| 29 | CH | 141 | LYS | 6.5 |
| 55 | DI | 20 | LYS | 6.5 |
| 26 | CE | 4 | VAL | 6.5 |
| 39 | CS | 33 | VAL | 6.5 |
| 2 | BB | 161 | LEU | 6.5 |
| 13 | BM | 95 | LEU | 6.5 |
| 53 | DA | 1065 | U | 6.5 |
| 9 | BI | 27 | LYS | 6.4 |
| 22 | CA | 2101 | A | 6.4 |
| 13 | BM | 38 | GLY | 6.4 |
| 26 | CE | 2 | GLU | 6.4 |
| 55 | DI | 11 | ILE | 6.4 |
| 55 | DI | 134 | GLU | 6.4 |
| 30 | CJ | 90 | SER | 6.4 |
| 9 | AI | 29 | VAL | 6.4 |
| 35 | CO | 38 | LEU | 6.4 |
| 36 | CP | 85 | LYS | 6.4 |
| 20 | BT | 65 | GLY | 6.4 |
| 55 | DI | 88 | HIS | 6.4 |
| 26 | CE | 108 | ILE | 6.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | CA | 344 | A | 6.4 |
| 26 | CE | 201 | ALA | 6.4 |
| 25 | CD | 184 | ARG | 6.4 |
| 33 | CM | 123 | ARG | 6.4 |
| 41 | CU | 76 | ARG | 6.4 |
| 3 | AC | 75 | ILE | 6.4 |
| 9 | BI | 20 | PHE | 6.4 |
| 2 | BB | 124 | GLY | 6.4 |
| 27 | CF | 21 | ASN | 6.4 |
| 7 | BG | 53 | ARG | 6.4 |
| 20 | BT | 7 | ALA | 6.4 |
| 2 | BB | 82 | ASP | 6.4 |
| 28 | CG | 20 | ASN | 6.4 |
| 28 | CG | 30 | ASN | 6.4 |
| 53 | DA | 2156 | G | 6.4 |
| 10 | BJ | 16 | ARG | 6.4 |
| 44 | CX | 55 | ARG | 6.4 |
| 10 | AJ | 86 | ALA | 6.4 |
| 29 | CH | 49 | ALA | 6.4 |
| 2 | BB | 138 | THR | 6.4 |
| 29 | DH | 96 | THR | 6.4 |
| 37 | CQ | 3 | ASN | 6.4 |
| 24 | CC | 237 | GLY | 6.4 |
| 43 | CW | 32 | GLY | 6.4 |
| 22 | CA | 1407 | G | 6.4 |
| 49 | C2 | 34 | LEU | 6.4 |
| 24 | CC | 242 | LYS | 6.3 |
| 27 | CF | 84 | PRO | 6.3 |
| 41 | CU | 36 | LYS | 6.3 |
| 22 | CA | 2402 | U | 6.3 |
| 26 | CE | 21 | ARG | 6.3 |
| 1 | BA | 1270 | G | 6.3 |
| 10 | BJ | 25 | ILE | 6.3 |
| 22 | CA | 2115 | G | 6.3 |
| 44 | CX | 60 | PHE | 6.3 |
| 22 | CA | 1871 | A | 6.3 |
| 24 | CC | 245 | VAL | 6.3 |
| 41 | CU | 85 | VAL | 6.3 |
| 30 | DJ | 73 | THR | 6.3 |
| 9 | BI | 62 | ASP | 6.3 |
| 7 | BG | 101 | MET | 6.3 |
| 13 | AM | 39 | ILE | 6.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 30 | CJ | 74 | PRO | 6.3 |
| 2 | AB | 35 | ARG | 6.3 |
| 39 | CS | 36 | ALA | 6.3 |
| 29 | CH | 6 | LEU | 6.3 |
| 29 | CH | 125 | THR | 6.3 |
| 2 | BB | 62 | SER | 6.3 |
| 22 | CA | 491 | G | 6.3 |
| 53 | DA | 2116 | G | 6.3 |
| 53 | DA | 2176 | A | 6.3 |
| 1 | AA | 1027 | C | 6.3 |
| 27 | CF | 78 | LYS | 6.3 |
| 44 | CX | 75 | LYS | 6.3 |
| 14 | BN | 44 | ALA | 6.3 |
| 29 | DH | 64 | ALA | 6.3 |
| 49 | C2 | 52 | ALA | 6.3 |
| 2 | BB | 14 | VAL | 6.3 |
| 7 | BG | 23 | LEU | 6.3 |
| 37 | CQ | 73 | VAL | 6.3 |
| 36 | CP | 65 | THR | 6.3 |
| 19 | BS | 4 | SER | 6.3 |
| 22 | CA | 1074 | G | 6.3 |
| 22 | CA | 1538 | G | 6.3 |
| 3 | BC | 103 | ILE | 6.3 |
| 28 | CG | 97 | ALA | 6.3 |
| 22 | CA | 1083 | U | 6.3 |
| 26 | CE | 196 | VAL | 6.3 |
| 9 | AI | 93 | SER | 6.3 |
| 28 | CG | 104 | ASN | 6.3 |
| 1 | BA | 206 | C | 6.3 |
| 22 | CA | 2107 | G | 6.3 |
| 22 | CA | 2159 | G | 6.3 |
| 53 | DA | 2178 | C | 6.3 |
| 10 | BJ | 39 | PRO | 6.3 |
| 30 | CJ | 52 | GLY | 6.3 |
| 36 | CP | 114 | GLY | 6.3 |
| 2 | AB | 75 | ALA | 6.3 |
| 26 | CE | 88 | ARG | 6.3 |
| 49 | C2 | 5 | ILE | 6.3 |
| 2 | AB | 221 | VAL | 6.2 |
| 25 | CD | 104 | VAL | 6.2 |
| 28 | CG | 116 | GLN | 6.2 |
| 37 | CQ | 7 | GLN | 6.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | BA | 94 | G | 6.2 |
| 28 | CG | 174 | ALA | 6.2 |
| 29 | CH | 63 | ALA | 6.2 |
| 19 | BS | 53 | ASN | 6.2 |
| 2 | BB | 213 | TYR | 6.2 |
| 49 | C2 | 48 | ILE | 6.2 |
| 46 | CZ | 18 | LEU | 6.2 |
| 2 | AB | 47 | VAL | 6.2 |
| 10 | BJ | 94 | ALA | 6.2 |
| 35 | CO | 59 | SER | 6.2 |
| 3 | BC | 196 | ILE | 6.2 |
| 49 | C2 | 27 | LYS | 6.2 |
| 2 | BB | 136 | MET | 6.2 |
| 3 | BC | 144 | LEU | 6.2 |
| 42 | CV | 14 | LEU | 6.2 |
| 1 | BA | 191 | G | 6.2 |
| 3 | BC | 39 | VAL | 6.2 |
| 39 | CS | 96 | VAL | 6.2 |
| 53 | DA | 1063 | G | 6.2 |
| 19 | AS | 8 | GLY | 6.2 |
| 7 | BG | 56 | LYS | 6.2 |
| 26 | CE | 26 | ALA | 6.2 |
| 35 | CO | 111 | ALA | 6.2 |
| 18 | AR | 74 | HIS | 6.2 |
| 49 | C2 | 31 | PRO | 6.2 |
| 1 | BA | 1266 | G | 6.2 |
| 1 | BA | 1312 | G | 6.2 |
| 9 | BI | 63 | LEU | 6.2 |
| 48 | C1 | 35 | GLY | 6.2 |
| 1 | BA | 1226 | C | 6.2 |
| 7 | BG | 122 | ASN | 6.2 |
| 29 | DH | 83 | LYS | 6.2 |
| 53 | DA | 2158 | A | 6.2 |
| 7 | AG | 83 | SER | 6.2 |
| 1 | BA | 942 | G | 6.2 |
| 22 | CA | 1211 | C | 6.2 |
| 2 | BB | 116 | ASP | 6.2 |
| 14 | AN | 27 | LEU | 6.2 |
| 11 | BK | 52 | PHE | 6.2 |
| 27 | CF | 146 | VAL | 6.2 |
| 6 | BF | 69 | GLU | 6.2 |
| 33 | CM | 106 | GLU | 6.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 22 | CA | 1075 | C | 6.1 |
| 27 | CF | 26 | MET | 6.1 |
| 40 | CT | 65 | ASP | 6.1 |
| 22 | CA | 2117 | A | 6.1 |
| 30 | CJ | 134 | ARG | 6.1 |
| 53 | DA | 2125 | G | 6.1 |
| 16 | BP | 54 | LEU | 6.1 |
| 43 | CW | 82 | TYR | 6.1 |
| 51 | C4 | 62 | LEU | 6.1 |
| 13 | BM | 52 | GLN | 6.1 |
| 55 | DI | 26 | VAL | 6.1 |
| 29 | DH | 140 | ALA | 6.1 |
| 36 | CP | 107 | ALA | 6.1 |
| 37 | CQ | 91 | ALA | 6.1 |
| 5 | BE | 146 | ASN | 6.1 |
| 28 | CG | 122 | THR | 6.1 |
| 29 | CH | 77 | THR | 6.1 |
| 25 | CD | 6 | GLY | 6.1 |
| 27 | CF | 144 | ASP | 6.1 |
| 22 | CA | 142 | A | 6.1 |
| 22 | CA | 279 | A | 6.1 |
| 53 | DA | 141 | G | 6.1 |
| 9 | AI | 59 | GLU | 6.1 |
| 47 | C0 | 32 | ILE | 6.1 |
| 22 | CA | 1100 | C | 6.1 |
| 29 | CH | 147 | VAL | 6.1 |
| 29 | DH | 132 | PHE | 6.1 |
| 36 | CP | 72 | ALA | 6.1 |
| 28 | CG | 34 | THR | 6.1 |
| 42 | CV | 78 | GLY | 6.1 |
| 8 | BH | 111 | MET | 6.1 |
| 1 | BA | 999 | C | 6.1 |
| 3 | BC | 127 | ARG | 6.1 |
| 14 | BN | 48 | LEU | 6.1 |
| 26 | CE | 191 | ASP | 6.1 |
| 41 | CU | 79 | ASP | 6.1 |
| 2 | BB | 128 | LYS | 6.1 |
| 3 | BC | 85 | GLU | 6.1 |
| 10 | AJ | 77 | VAL | 6.1 |
| 11 | BK | 73 | ALA | 6.1 |
| 28 | CG | 113 | VAL | 6.1 |
| 51 | C4 | 15 | LYS | 6.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | BA | 1357 | A | 6.1 |
| 22 | CA | 356 | G | 6.1 |
| 22 | CA | 1091 | G | 6.1 |
| 35 | CO | 27 | SER | 6.1 |
| 1 | AA | 87 | C | 6.1 |
| 7 | BG | 4 | ARG | 6.1 |
| 23 | CB | 37 | C | 6.1 |
| 55 | DI | 98 | GLU | 6.1 |
| 22 | CA | 1066 | U | 6.1 |
| 17 | BQ | 56 | GLY | 6.1 |
| 24 | CC | 34 | LEU | 6.1 |
| 28 | CG | 57 | GLY | 6.1 |
| 2 | BB | 84 | ALA | 6.1 |
| 13 | BM | 18 | ALA | 6.1 |
| 51 | C4 | 37 | ALA | 6.1 |
| 51 | C4 | 60 | ALA | 6.1 |
| 10 | BJ | 32 | THR | 6.1 |
| 1 | BA | 1356 | G | 6.1 |
| 42 | CV | 9 | ASP | 6.1 |
| 53 | DA | 1064 | C | 6.1 |
| 27 | CF | 63 | GLN | 6.1 |
| 37 | CQ | 23 | GLY | 6.1 |
| 51 | C4 | 18 | GLY | 6.1 |
| 55 | DI | 49 | GLY | 6.1 |
| 2 | AB | 134 | ALA | 6.1 |
| 7 | AG | 46 | ALA | 6.1 |
| 9 | AI | 28 | ILE | 6.1 |
| 24 | CC | 33 | LEU | 6.1 |
| 36 | CP | 35 | ILE | 6.1 |
| 40 | CT | 63 | GLY | 6.0 |
| 50 | C3 | 33 | ARG | 6.0 |
| 55 | DI | 43 | LYS | 6.0 |
| 1 | AA | 83 | C | 6.0 |
| 1 | AA | 1031 | C | 6.0 |
| 1 | BA | 1265 | C | 6.0 |
| 9 | BI | 61 | LEU | 6.0 |
| 22 | CA | 1044 | C | 6.0 |
| 55 | DI | 135 | ALA | 6.0 |
| 29 | CH | 132 | PHE | 6.0 |
| 42 | CV | 95 | PHE | 6.0 |
| 22 | CA | 1042 | G | 6.0 |
| 1 | AA | 1534 | A | 6.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 13 | BM | 3 | ARG | 6.0 |
| 27 | DF | 113 | ASP | 6.0 |
| 52 | C5 | 20 | ASP | 6.0 |
| 10 | BJ | 23 | ALA | 6.0 |
| 30 | DJ | 84 | ALA | 6.0 |
| 1 | BA | 5 | U | 6.0 |
| 53 | DA | 2181 | U | 6.0 |
| 26 | CE | 120 | VAL | 6.0 |
| 9 | BI | 45 | ARG | 6.0 |
| 33 | CM | 126 | ARG | 6.0 |
| 37 | CQ | 16 | ASP | 6.0 |
| 30 | CJ | 111 | GLN | 6.0 |
| 35 | CO | 73 | ASN | 6.0 |
| 29 | CH | 36 | ALA | 6.0 |
| 55 | DI | 133 | GLU | 6.0 |
| 10 | BJ | 10 | LEU | 6.0 |
| 13 | AM | 34 | LEU | 6.0 |
| 13 | BM | 56 | LEU | 6.0 |
| 13 | AM | 53 | ILE | 6.0 |
| 22 | CA | 2157 | G | 6.0 |
| 5 | BE | 91 | GLY | 6.0 |
| 24 | CC | 120 | VAL | 6.0 |
| 30 | DJ | 29 | GLY | 6.0 |
| 30 | DJ | 70 | VAL | 6.0 |
| 19 | BS | 52 | HIS | 6.0 |
| 6 | BF | 92 | THR | 6.0 |
| 36 | CP | 73 | ALA | 6.0 |
| 1 | AA | 412 | A | 6.0 |
| 41 | CU | 11 | LEU | 6.0 |
| 9 | BI | 64 | TYR | 6.0 |
| 17 | BQ | 79 | VAL | 6.0 |
| 28 | CG | 98 | VAL | 6.0 |
| 43 | CW | 72 | VAL | 6.0 |
| 7 | AG | 151 | PHE | 6.0 |
| 6 | BF | 91 | ARG | 6.0 |
| 22 | CA | 139 | U | 6.0 |
| 53 | DA | 139 | U | 6.0 |
| 38 | CR | 10 | ALA | 6.0 |
| 27 | CF | 94 | GLU | 6.0 |
| 27 | CF | 82 | GLY | 6.0 |
| 53 | DA | 2162 | G | 6.0 |
| 20 | BT | 32 | ILE | 6.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 22 | CA | 547 | A | 5.9 |
| 2 | AB | 130 | THR | 5.9 |
| 2 | BB | 37 | LYS | 5.9 |
| 31 | CK | 131 | ASN | 5.9 |
| 10 | BJ | 41 | PRO | 5.9 |
| 28 | CG | 85 | LYS | 5.9 |
| 53 | DA | 2126 | A | 5.9 |
| 43 | CW | 1 | MET | 5.9 |
| 9 | BI | 16 | ALA | 5.9 |
| 20 | BT | 87 | ALA | 5.9 |
| 1 | BA | 1246 | A | 5.9 |
| 16 | BP | 60 | TRP | 5.9 |
| 22 | CA | 2305 | U | 5.9 |
| 27 | CF | 89 | VAL | 5.9 |
| 28 | CG | 129 | THR | 5.9 |
| 40 | CT | 99 | ARG | 5.9 |
| 2 | BB | 91 | PHE | 5.9 |
| 7 | BG | 123 | GLU | 5.9 |
| 1 | AA | 1020 | G | 5.9 |
| 33 | CM | 91 | ASP | 5.9 |
| 7 | AG | 13 | LEU | 5.9 |
| 29 | CH | 11 | ASN | 5.9 |
| 11 | BK | 74 | VAL | 5.9 |
| 13 | BM | 20 | THR | 5.9 |
| 33 | CM | 130 | GLY | 5.9 |
| 36 | CP | 74 | VAL | 5.9 |
| 49 | C2 | 29 | THR | 5.9 |
| 1 | BA | 1286 | U | 5.9 |
| 53 | DA | 1176 | U | 5.9 |
| 53 | DA | 2172 | U | 5.9 |
| 36 | CP | 108 | ASP | 5.9 |
| 22 | CA | 2146 | C | 5.9 |
| 33 | CM | 68 | SER | 5.9 |
| 9 | BI | 92 | GLU | 5.9 |
| 10 | BJ | 89 | ARG | 5.9 |
| 35 | CO | 46 | ARG | 5.9 |
| 28 | CG | 48 | ASN | 5.9 |
| 27 | CF | 64 | LYS | 5.9 |
| 36 | CP | 18 | LEU | 5.9 |
| 36 | CP | 38 | GLN | 5.9 |
| 21 | AU | 57 | ALA | 5.9 |
| 30 | DJ | 35 | ILE | 5.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 24 | CC | 213 | TRP | 5.9 |
| 22 | CA | 2799 | A | 5.9 |
| 43 | CW | 56 | PHE | 5.9 |
| 22 | CA | 1112 | G | 5.9 |
| 41 | CU | 49 | LYS | 5.9 |
| 9 | AI | 24 | GLY | 5.9 |
| 55 | DI | 52 | MET | 5.9 |
| 9 | BI | 53 | GLU | 5.8 |
| 30 | CJ | 123 | GLU | 5.8 |
| 55 | DI | 114 | GLU | 5.8 |
| 2 | BB | 41 | ILE | 5.8 |
| 7 | AG | 56 | LYS | 5.8 |
| 29 | DH | 67 | ALA | 5.8 |
| 42 | CV | 72 | ILE | 5.8 |
| 26 | CE | 151 | GLY | 5.8 |
| 40 | CT | 67 | ASP | 5.8 |
| 2 | AB | 74 | ARG | 5.8 |
| 9 | BI | 22 | LYS | 5.8 |
| 26 | CE | 137 | LYS | 5.8 |
| 2 | BB | 212 | LEU | 5.8 |
| 26 | CE | 200 | LEU | 5.8 |
| 22 | CA | 2176 | A | 5.8 |
| 43 | CW | 84 | PRO | 5.8 |
| 36 | CP | 113 | ALA | 5.8 |
| 16 | BP | 78 | VAL | 5.8 |
| 21 | AU | 4 | ILE | 5.8 |
| 46 | CZ | 14 | LEU | 5.8 |
| 22 | CA | 1047 | G | 5.8 |
| 2 | BB | 156 | GLY | 5.8 |
| 22 | CA | 2179 | C | 5.8 |
| 28 | CG | 164 | TYR | 5.8 |
| 1 | AA | 1025 | U | 5.8 |
| 22 | CA | 1174 | U | 5.8 |
| 9 | BI | 86 | ALA | 5.8 |
| 10 | AJ | 34 | ALA | 5.8 |
| 14 | AN | 40 | ASP | 5.8 |
| 29 | DH | 59 | ALA | 5.8 |
| 10 | BJ | 9 | ARG | 5.8 |
| 1 | BA | 846 | G | 5.8 |
| 1 | BA | 1355 | G | 5.8 |
| 7 | AG | 91 | VAL | 5.8 |
| 9 | BI | 65 | ILE | 5.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 11 | AK | 113 | VAL | 5.8 |
| 33 | CM | 77 | ILE | 5.8 |
| 40 | CT | 45 | VAL | 5.8 |
| 55 | DI | 87 | GLU | 5.8 |
| 22 | CA | 1057 | A | 5.8 |
| 3 | BC | 42 | TYR | 5.8 |
| 51 | C4 | 2 | PRO | 5.8 |
| 10 | BJ | 31 | ARG | 5.8 |
| 29 | CH | 27 | ARG | 5.8 |
| 2 | BB | 216 | ALA | 5.8 |
| 10 | BJ | 29 | ALA | 5.8 |
| 20 | AT | 47 | ALA | 5.8 |
| 2 | AB | 215 | GLY | 5.8 |
| 25 | CD | 158 | GLY | 5.8 |
| 36 | CP | 112 | GLU | 5.8 |
| 22 | CA | 2802 | G | 5.8 |
| 22 | CA | 2602 | A | 5.8 |
| 26 | CE | 187 | VAL | 5.8 |
| 50 | C3 | 22 | MET | 5.8 |
| 19 | AS | 9 | PRO | 5.8 |
| 39 | CS | 93 | PHE | 5.8 |
| 1 | BA | 1314 | C | 5.8 |
| 50 | C3 | 27 | GLY | 5.7 |
| 22 | CA | 342 | A | 5.7 |
| 22 | CA | 1869 | G | 5.7 |
| 41 | CU | 28 | ASN | 5.7 |
| 22 | CA | 1078 | U | 5.7 |
| 24 | CC | 77 | VAL | 5.7 |
| 45 | CY | 67 | VAL | 5.7 |
| 48 | C1 | 25 | VAL | 5.7 |
| 44 | CX | 52 | GLY | 5.7 |
| 1 | BA | 1302 | C | 5.7 |
| 13 | BM | 53 | ILE | 5.7 |
| 29 | CH | 72 | ILE | 5.7 |
| 5 | BE | 157 | ARG | 5.7 |
| 16 | AP | 82 | ALA | 5.7 |
| 26 | CE | 154 | ASP | 5.7 |
| 29 | CH | 59 | ALA | 5.7 |
| 30 | CJ | 47 | ASP | 5.7 |
| 30 | CJ | 127 | ARG | 5.7 |
| 50 | C3 | 37 | LYS | 5.7 |
| 53 | DA | 2124 | G | 5.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 26 | CE | 157 | LEU | 5.7 |
| 30 | DJ | 74 | PRO | 5.7 |
| 43 | CW | 48 | MET | 5.7 |
| 6 | BF | 20 | GLY | 5.7 |
| 1 | BA | 1000 | A | 5.7 |
| 38 | CR | 30 | ARG | 5.7 |
| 2 | BB | 134 | ALA | 5.7 |
| 3 | BC | 104 | ALA | 5.7 |
| 7 | BG | 149 | LYS | 5.7 |
| 22 | CA | 1099 | G | 5.7 |
| 22 | CA | 1168 | G | 5.7 |
| 26 | CE | 10 | SER | 5.7 |
| 36 | CP | 115 | LEU | 5.7 |
| 41 | CU | 4 | GLU | 5.7 |
| 13 | BM | 57 | ARG | 5.7 |
| 16 | AP | 46 | LYS | 5.7 |
| 11 | BK | 44 | TRP | 5.7 |
| 2 | BB | 111 | ILE | 5.7 |
| 17 | BQ | 55 | ILE | 5.7 |
| 43 | CW | 89 | ILE | 5.7 |
| 36 | CP | 14 | ALA | 5.7 |
| 1 | BA | 1310 | G | 5.7 |
| 3 | AC | 168 | TYR | 5.7 |
| 10 | BJ | 24 | GLU | 5.7 |
| 17 | BQ | 75 | LEU | 5.7 |
| 22 | CA | 2173 | A | 5.7 |
| 41 | CU | 15 | HIS | 5.7 |
| 2 | BB | 220 | THR | 5.7 |
| 4 | AD | 160 | GLU | 5.7 |
| 10 | BJ | 35 | GLN | 5.7 |
| 27 | CF | 74 | VAL | 5.7 |
| 34 | CN | 80 | VAL | 5.7 |
| 42 | CV | 70 | VAL | 5.7 |
| 2 | BB | 53 | ALA | 5.7 |
| 43 | CW | 6 | ALA | 5.7 |
| 44 | CX | 84 | ALA | 5.7 |
| 55 | DI | 48 | ALA | 5.7 |
| 13 | BM | 76 | SER | 5.6 |
| 28 | CG | 73 | ASN | 5.6 |
| 22 | CA | 2103 | C | 5.6 |
| 23 | CB | 118 | C | 5.6 |
| 25 | CD | 187 | LEU | 5.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | DH | 117 | LEU | 5.6 |
| 19 | BS | 33 | THR | 5.6 |
| 2 | BB | 218 | ALA | 5.6 |
| 11 | BK | 63 | ALA | 5.6 |
| 32 | CL | 115 | ILE | 5.6 |
| 22 | CA | 1056 | G | 5.6 |
| 7 | BG | 116 | MET | 5.6 |
| 9 | AI | 97 | GLU | 5.6 |
| 46 | CZ | 8 | GLU | 5.6 |
| 3 | AC | 78 | GLY | 5.6 |
| 28 | CG | 14 | GLY | 5.6 |
| 40 | CT | 3 | THR | 5.6 |
| 10 | AJ | 36 | VAL | 5.6 |
| 22 | CA | 2803 | G | 5.6 |
| 15 | BO | 11 | ILE | 5.6 |
| 3 | BC | 167 | TRP | 5.6 |
| 20 | BT | 43 | ASP | 5.6 |
| 29 | DH | 58 | LEU | 5.6 |
| 47 | C0 | 24 | LEU | 5.6 |
| 1 | AA | 1 | A | 5.6 |
| 30 | DJ | 83 | ALA | 5.6 |
| 35 | CO | 85 | PRO | 5.6 |
| 2 | BB | 208 | ARG | 5.6 |
| 3 | AC | 39 | VAL | 5.6 |
| 30 | DJ | 136 | MET | 5.6 |
| 53 | DA | 2127 | G | 5.6 |
| 28 | CG | 166 | ASP | 5.6 |
| 30 | DJ | 60 | THR | 5.6 |
| 2 | BB | 109 | GLN | 5.6 |
| 42 | CV | 61 | LYS | 5.6 |
| 49 | C2 | 30 | LYS | 5.6 |
| 53 | DA | 1067 | A | 5.6 |
| 4 | BD | 47 | ARG | 5.6 |
| 11 | BK | 71 | ALA | 5.6 |
| 42 | CV | 22 | ARG | 5.6 |
| 36 | CP | 66 | GLY | 5.6 |
| 22 | CA | 1731 | G | 5.6 |
| 28 | CG | 167 | GLU | 5.6 |
| 29 | DH | 66 | ASN | 5.6 |
| 9 | AI | 60 | LYS | 5.6 |
| 17 | BQ | 7 | THR | 5.6 |
| 2 | AB | 226 | SER | 5.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 53 | DA | 2161 | C | 5.6 |
| 14 | BN | 69 | ARG | 5.6 |
| 53 | DA | 2169 | A | 5.6 |
| 7 | BG | 99 | LEU | 5.6 |
| 9 | BI | 52 | LEU | 5.6 |
| 25 | CD | 31 | ALA | 5.6 |
| 53 | DA | 2167 | U | 5.6 |
| 22 | CA | 2124 | G | 5.6 |
| 47 | C0 | 56 | LYS | 5.5 |
| 22 | CA | 893 | C | 5.5 |
| 26 | CE | 16 | GLU | 5.5 |
| 42 | CV | 86 | ARG | 5.5 |
| 30 | CJ | 132 | THR | 5.5 |
| 33 | CM | 74 | THR | 5.5 |
| 53 | DA | 896 | A | 5.5 |
| 55 | DI | 89 | PRO | 5.5 |
| 2 | BB | 39 | HIS | 5.5 |
| 7 | AG | 18 | PHE | 5.5 |
| 41 | CU | 32 | LEU | 5.5 |
| 31 | CK | 1 | MET | 5.5 |
| 1 | BA | 1142 | G | 5.5 |
| 15 | AO | 17 | ARG | 5.5 |
| 22 | CA | 1523 | U | 5.5 |
| 1 | BA | 1271 | A | 5.5 |
| 17 | BQ | 59 | VAL | 5.5 |
| 29 | CH | 131 | SER | 5.5 |
| 6 | BF | 31 | GLY | 5.5 |
| 9 | BI | 56 | ASP | 5.5 |
| 9 | BI | 4 | ASN | 5.5 |
| 14 | BN | 46 | LEU | 5.5 |
| 20 | AT | 50 | ALA | 5.5 |
| 33 | CM | 71 | ALA | 5.5 |
| 22 | CA | 2175 | C | 5.5 |
| 27 | CF | 178 | ARG | 5.5 |
| 28 | CG | 95 | ARG | 5.5 |
| 53 | DA | 356 | G | 5.5 |
| 1 | AA | 845 | A | 5.5 |
| 26 | CE | 55 | SER | 5.5 |
| 36 | CP | 88 | LYS | 5.5 |
| 28 | CG | 4 | VAL | 5.5 |
| 19 | BS | 81 | ARG | 5.5 |
| 1 | BA | 1279 | G | 5.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 9 | AI | 63 | LEU | 5.5 |
| 28 | CG | 117 | LEU | 5.5 |
| 31 | CK | 125 | TYR | 5.5 |
| 22 | CA | 1090 | A | 5.5 |
| 20 | BT | 82 | GLN | 5.5 |
| 27 | CF | 134 | GLU | 5.5 |
| 9 | AI | 55 | VAL | 5.5 |
| 1 | BA | 90 | C | 5.5 |
| 1 | BA | 1132 | C | 5.5 |
| 42 | CV | 79 | LYS | 5.5 |
| 9 | AI | 65 | ILE | 5.5 |
| 29 | DH | 72 | ILE | 5.5 |
| 7 | BG | 108 | ALA | 5.5 |
| 50 | C3 | 32 | ALA | 5.5 |
| 1 | BA | 1292 | G | 5.5 |
| 1 | BA | 1491 | G | 5.5 |
| 22 | CA | 1873 | G | 5.5 |
| 53 | DA | 549 | G | 5.5 |
| 8 | AH | 2 | SER | 5.5 |
| 9 | BI | 94 | LEU | 5.5 |
| 13 | BM | 54 | ASP | 5.5 |
| 28 | CG | 87 | LEU | 5.5 |
| 35 | CO | 94 | TYR | 5.5 |
| 20 | BT | 84 | ASN | 5.5 |
| 46 | CZ | 20 | ASN | 5.5 |
| 35 | CO | 56 | LYS | 5.5 |
| 53 | DA | 1730 | C | 5.5 |
| 53 | DA | 2179 | C | 5.5 |
| 11 | AK | 110 | ILE | 5.5 |
| 19 | BS | 75 | ALA | 5.5 |
| 38 | CR | 35 | ALA | 5.5 |
| 39 | CS | 26 | ASP | 5.5 |
| 22 | CA | 277 | G | 5.5 |
| 22 | CA | 1734 | G | 5.5 |
| 11 | AK | 96 | THR | 5.4 |
| 30 | DJ | 112 | THR | 5.4 |
| 48 | C1 | 33 | THR | 5.4 |
| 1 | AA | 1492 | A | 5.4 |
| 1 | BA | 460 | A | 5.4 |
| 2 | AB | 123 | ASP | 5.4 |
| 25 | CD | 155 | VAL | 5.4 |
| 26 | CE | 178 | VAL | 5.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 48 | C1 | 46 | ASP | 5.4 |
| 1 | BA | 1026 | G | 5.4 |
| 17 | BQ | 20 | SER | 5.4 |
| 29 | DH | 49 | ALA | 5.4 |
| 22 | CA | 438 | G | 5.4 |
| 27 | CF | 44 | ILE | 5.4 |
| 26 | CE | 174 | GLY | 5.4 |
| 19 | AS | 10 | PHE | 5.4 |
| 35 | CO | 102 | PHE | 5.4 |
| 22 | CA | 282 | A | 5.4 |
| 53 | DA | 1089 | A | 5.4 |
| 3 | BC | 84 | VAL | 5.4 |
| 28 | CG | 74 | SER | 5.4 |
| 32 | CL | 69 | VAL | 5.4 |
| 33 | CM | 46 | VAL | 5.4 |
| 44 | CX | 31 | VAL | 5.4 |
| 6 | BF | 94 | HIS | 5.4 |
| 11 | BK | 51 | GLY | 5.4 |
| 3 | BC | 33 | LEU | 5.4 |
| 17 | BQ | 81 | LYS | 5.4 |
| 13 | BM | 102 | THR | 5.4 |
| 5 | BE | 10 | GLU | 5.4 |
| 31 | CK | 129 | GLU | 5.4 |
| 39 | CS | 46 | GLU | 5.4 |
| 1 | BA | 213 | G | 5.4 |
| 13 | AM | 37 | ALA | 5.4 |
| 29 | CH | 56 | ALA | 5.4 |
| 36 | CP | 90 | VAL | 5.4 |
| 9 | BI | 50 | GLN | 5.4 |
| 14 | BN | 72 | GLY | 5.4 |
| 9 | BI | 120 | LYS | 5.4 |
| 14 | BN | 23 | LYS | 5.4 |
| 8 | BH | 46 | ILE | 5.4 |
| 6 | BF | 39 | LEU | 5.4 |
| 7 | AG | 59 | LEU | 5.4 |
| 27 | CF | 165 | GLU | 5.4 |
| 34 | CN | 54 | THR | 5.4 |
| 40 | CT | 97 | LEU | 5.4 |
| 43 | CW | 42 | LEU | 5.4 |
| 3 | BC | 130 | PHE | 5.4 |
| 22 | CA | 436 | C | 5.4 |
| 16 | BP | 76 | LYS | 5.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | AC | 83 | ASP | 5.4 |
| 17 | BQ | 48 | ASP | 5.4 |
| 19 | AS | 22 | ALA | 5.4 |
| 20 | BT | 38 | ALA | 5.4 |
| 27 | CF | 46 | ASP | 5.4 |
| 1 | BA | 1274 | A | 5.4 |
| 22 | CA | 44 | A | 5.4 |
| 30 | CJ | 122 | ILE | 5.4 |
| 48 | C1 | 55 | ILE | 5.4 |
| 22 | CA | 280 | U | 5.4 |
| 28 | CG | 50 | LEU | 5.4 |
| 28 | CG | 153 | ARG | 5.4 |
| 34 | CN | 61 | GLY | 5.4 |
| 26 | CE | 135 | ALA | 5.4 |
| 28 | CG | 12 | PRO | 5.4 |
| 50 | C3 | 7 | PRO | 5.4 |
| 1 | AA | 205 | A | 5.4 |
| 29 | CH | 138 | VAL | 5.4 |
| 2 | BB | 58 | ASN | 5.4 |
| 7 | BG | 137 | LYS | 5.4 |
| 27 | CF | 23 | ASN | 5.4 |
| 28 | CG | 172 | LYS | 5.4 |
| 37 | CQ | 5 | ILE | 5.3 |
| 2 | BB | 7 | ARG | 5.3 |
| 7 | BG | 13 | LEU | 5.3 |
| 39 | CS | 25 | LEU | 5.3 |
| 41 | CU | 5 | GLU | 5.3 |
| 42 | CV | 84 | GLY | 5.3 |
| 22 | CA | 2126 | A | 5.3 |
| 26 | CE | 34 | ALA | 5.3 |
| 35 | CO | 88 | ALA | 5.3 |
| 36 | CP | 32 | PRO | 5.3 |
| 10 | AJ | 98 | VAL | 5.3 |
| 27 | CF | 42 | GLU | 5.3 |
| 2 | BB | 35 | ARG | 5.3 |
| 26 | CE | 179 | SER | 5.3 |
| 22 | CA | 2167 | U | 5.3 |
| 53 | DA | 546 | U | 5.3 |
| 10 | AJ | 18 | ILE | 5.3 |
| 13 | AM | 7 | ILE | 5.3 |
| 15 | BO | 82 | ILE | 5.3 |
| 38 | CR | 23 | GLY | 5.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | BA | 1012 | A | 5.3 |
| 11 | BK | 47 | ALA | 5.3 |
| 16 | AP | 72 | ALA | 5.3 |
| 22 | CA | 141 | G | 5.3 |
| 28 | CG | 22 | GLN | 5.3 |
| 53 | DA | 2123 | G | 5.3 |
| 36 | CP | 81 | ARG | 5.3 |
| 16 | BP | 44 | SER | 5.3 |
| 31 | CK | 17 | VAL | 5.3 |
| 40 | CT | 105 | VAL | 5.3 |
| 26 | CE | 103 | GLY | 5.3 |
| 2 | BB | 49 | MET | 5.3 |
| 19 | AS | 65 | GLU | 5.3 |
| 53 | DA | 1069 | A | 5.3 |
| 29 | DH | 145 | ASN | 5.3 |
| 35 | CO | 10 | LEU | 5.3 |
| 52 | C5 | 13 | ASN | 5.3 |
| 22 | CA | 405 | U | 5.3 |
| 22 | CA | 2904 | U | 5.3 |
| 4 | AD | 27 | ALA | 5.3 |
| 22 | CA | 359 | G | 5.3 |
| 55 | DI | 125 | ARG | 5.3 |
| 46 | CZ | 16 | THR | 5.3 |
| 2 | BB | 44 | GLU | 5.3 |
| 10 | BJ | 81 | GLU | 5.3 |
| 36 | CP | 28 | VAL | 5.3 |
| 49 | C2 | 16 | GLY | 5.3 |
| 1 | BA | 1293 | C | 5.3 |
| 53 | DA | 2109 | U | 5.3 |
| 7 | AG | 109 | ARG | 5.3 |
| 8 | BH | 54 | ASP | 5.3 |
| 19 | AS | 16 | LEU | 5.3 |
| 27 | CF | 145 | LYS | 5.3 |
| 28 | CG | 56 | ASP | 5.3 |
| 22 | CA | 276 | U | 5.3 |
| 25 | CD | 151 | THR | 5.3 |
| 1 | BA | 1492 | A | 5.3 |
| 32 | CL | 90 | ASN | 5.3 |
| 8 | BH | 39 | VAL | 5.3 |
| 25 | CD | 26 | VAL | 5.3 |
| 28 | CG | 62 | TRP | 5.3 |
| 2 | AB | 82 | ASP | 5.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 30 | DJ | 10 | LYS | 5.3 |
| 9 | AI | 32 | GLN | 5.3 |
| 1 | BA | 1303 | C | 5.3 |
| 33 | CM | 30 | THR | 5.3 |
| 35 | CO | 57 | THR | 5.3 |
| 1 | BA | 843 | U | 5.3 |
| 10 | BJ | 79 | PRO | 5.3 |
| 13 | BM | 47 | GLU | 5.3 |
| 28 | CG | 162 | VAL | 5.2 |
| 1 | BA | 1241 | G | 5.2 |
| 22 | CA | 291 | G | 5.2 |
| 22 | CA | 406 | G | 5.2 |
| 23 | CB | 117 | G | 5.2 |
| 44 | CX | 25 | ARG | 5.2 |
| 7 | BG | 130 | ASN | 5.2 |
| 22 | CA | 1089 | A | 5.2 |
| 25 | CD | 118 | PHE | 5.2 |
| 31 | CK | 21 | THR | 5.2 |
| 28 | CG | 151 | TYR | 5.2 |
| 43 | CW | 68 | LYS | 5.2 |
| 46 | CZ | 54 | LYS | 5.2 |
| 7 | BG | 60 | GLU | 5.2 |
| 10 | BJ | 12 | ALA | 5.2 |
| 2 | AB | 151 | ILE | 5.2 |
| 40 | CT | 35 | ILE | 5.2 |
| 2 | AB | 32 | PHE | 5.2 |
| 51 | C4 | 14 | PHE | 5.2 |
| 7 | AG | 11 | LYS | 5.2 |
| 9 | BI | 123 | ARG | 5.2 |
| 49 | C2 | 21 | TYR | 5.2 |
| 45 | CY | 76 | GLU | 5.2 |
| 20 | BT | 70 | ASN | 5.2 |
| 55 | DI | 18 | VAL | 5.2 |
| 22 | CA | 1098 | A | 5.2 |
| 1 | BA | 1018 | G | 5.2 |
| 7 | BG | 19 | GLY | 5.2 |
| 34 | CN | 23 | GLY | 5.2 |
| 2 | AB | 186 | ILE | 5.2 |
| 14 | AN | 47 | LYS | 5.2 |
| 1 | AA | 84 | U | 5.2 |
| 28 | CG | 130 | GLU | 5.2 |
| 30 | CJ | 103 | ARG | 5.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 53 | DA | 1870 | C | 5.2 |
| 9 | BI | 31 | ASN | 5.2 |
| 1 | BA | 1441 | A | 5.2 |
| 38 | CR | 29 | SER | 5.2 |
| 22 | CA | 283 | G | 5.2 |
| 22 | CA | 315 | G | 5.2 |
| 29 | DH | 144 | VAL | 5.2 |
| 34 | CN | 135 | VAL | 5.2 |
| 2 | BB | 131 | LYS | 5.2 |
| 2 | AB | 227 | GLN | 5.2 |
| 21 | BU | 15 | ALA | 5.2 |
| 26 | CE | 142 | ALA | 5.2 |
| 27 | CF | 150 | ARG | 5.2 |
| 30 | CJ | 141 | GLU | 5.2 |
| 2 | BB | 157 | LEU | 5.2 |
| 17 | BQ | 41 | THR | 5.2 |
| 19 | BS | 5 | LEU | 5.2 |
| 29 | CH | 75 | LEU | 5.2 |
| 37 | CQ | 8 | LEU | 5.2 |
| 46 | CZ | 55 | THR | 5.2 |
| 37 | CQ | 63 | LYS | 5.2 |
| 2 | AB | 13 | GLY | 5.2 |
| 9 | BI | 90 | TYR | 5.2 |
| 53 | DA | 881 | G | 5.2 |
| 10 | AJ | 89 | ARG | 5.2 |
| 14 | BN | 11 | VAL | 5.2 |
| 7 | BG | 71 | PRO | 5.2 |
| 46 | CZ | 41 | HIS | 5.2 |
| 26 | CE | 188 | MET | 5.2 |
| 5 | AE | 164 | ILE | 5.2 |
| 46 | CZ | 24 | GLU | 5.2 |
| 1 | BA | 1365 | G | 5.1 |
| 22 | CA | 2122 | U | 5.1 |
| 29 | DH | 39 | ALA | 5.1 |
| 40 | CT | 32 | ALA | 5.1 |
| 9 | BI | 55 | VAL | 5.1 |
| 42 | CV | 11 | VAL | 5.1 |
| 9 | BI | 23 | PRO | 5.1 |
| 12 | BL | 44 | LYS | 5.1 |
| 22 | CA | 172 | A | 5.1 |
| 25 | CD | 199 | SER | 5.1 |
| 43 | CW | 38 | LEU | 5.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 28 | CG | 24 | ILE | 5.1 |
| 1 | AA | 842 | U | 5.1 |
| 44 | CX | 68 | LYS | 5.1 |
| 53 | DA | 2157 | G | 5.1 |
| 28 | CG | 111 | HIS | 5.1 |
| 19 | AS | 30 | PRO | 5.1 |
| 1 | BA | 1306 | A | 5.1 |
| 13 | AM | 52 | GLN | 5.1 |
| 22 | CA | 1111 | A | 5.1 |
| 24 | CC | 204 | VAL | 5.1 |
| 38 | CR | 104 | VAL | 5.1 |
| 41 | CU | 39 | THR | 5.1 |
| 55 | DI | 122 | GLN | 5.1 |
| 7 | BG | 37 | SER | 5.1 |
| 26 | CE | 67 | ARG | 5.1 |
| 32 | CL | 75 | SER | 5.1 |
| 17 | AQ | 55 | ILE | 5.1 |
| 7 | BG | 48 | GLU | 5.1 |
| 18 | AR | 20 | GLU | 5.1 |
| 26 | CE | 171 | ASP | 5.1 |
| 28 | CG | 32 | GLU | 5.1 |
| 43 | CW | 43 | ASP | 5.1 |
| 22 | CA | 880 | G | 5.1 |
| 7 | BG | 121 | ALA | 5.1 |
| 27 | CF | 29 | PRO | 5.1 |
| 31 | CK | 126 | ALA | 5.1 |
| 42 | CV | 2 | ALA | 5.1 |
| 45 | CY | 21 | ALA | 5.1 |
| 48 | C1 | 24 | ALA | 5.1 |
| 3 | BC | 44 | THR | 5.1 |
| 5 | BE | 159 | LYS | 5.1 |
| 13 | AM | 31 | LYS | 5.1 |
| 26 | CE | 169 | VAL | 5.1 |
| 2 | AB | 124 | GLY | 5.1 |
| 28 | CG | 28 | GLY | 5.1 |
| 29 | DH | 88 | GLY | 5.1 |
| 49 | C2 | 35 | GLU | 5.1 |
| 29 | DH | 12 | LEU | 5.1 |
| 20 | BT | 57 | ILE | 5.1 |
| 26 | CE | 41 | GLN | 5.1 |
| 46 | CZ | 31 | GLN | 5.1 |
| 22 | CA | 2100 | G | 5.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 53 | DA | 2100 | G | 5.1 |
| 1 | BA | 80 | A | 5.1 |
| 27 | CF | 9 | LYS | 5.1 |
| 27 | CF | 161 | LYS | 5.1 |
| 38 | CR | 84 | LYS | 5.1 |
| 44 | CX | 61 | ALA | 5.1 |
| 7 | AG | 26 | PHE | 5.1 |
| 7 | AG | 45 | SER | 5.1 |
| 37 | CQ | 57 | SER | 5.1 |
| 7 | BG | 91 | VAL | 5.1 |
| 9 | BI | 111 | VAL | 5.1 |
| 13 | AM | 58 | ASP | 5.1 |
| 45 | CY | 4 | VAL | 5.1 |
| 22 | CA | 846 | U | 5.1 |
| 47 | C0 | 3 | LYS | 5.1 |
| 1 | BA | 86 | G | 5.1 |
| 53 | DA | 2112 | G | 5.1 |
| 2 | AB | 53 | ALA | 5.1 |
| 10 | AJ | 75 | ASP | 5.1 |
| 7 | BG | 97 | ASN | 5.1 |
| 3 | BC | 40 | ARG | 5.1 |
| 21 | BU | 33 | ARG | 5.1 |
| 42 | CV | 67 | VAL | 5.1 |
| 51 | C4 | 23 | LYS | 5.1 |
| 41 | CU | 52 | GLU | 5.1 |
| 1 | AA | 1493 | A | 5.1 |
| 1 | BA | 1038 | C | 5.1 |
| 22 | CA | 1723 | G | 5.1 |
| 13 | BM | 73 | ILE | 5.0 |
| 37 | CQ | 84 | ILE | 5.0 |
| 2 | BB | 132 | LYS | 5.0 |
| 8 | BH | 55 | THR | 5.0 |
| 20 | BT | 8 | LYS | 5.0 |
| 26 | CE | 17 | THR | 5.0 |
| 1 | BA | 958 | A | 5.0 |
| 22 | CA | 2164 | C | 5.0 |
| 2 | AB | 43 | LEU | 5.0 |
| 2 | AB | 129 | LEU | 5.0 |
| 41 | CU | 40 | LYS | 5.0 |
| 14 | AN | 26 | GLU | 5.0 |
| 15 | BO | 7 | ALA | 5.0 |
| 26 | CE | 24 | ASN | 5.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | CH | 92 | GLY | 5.0 |
| 29 | DH | 100 | ALA | 5.0 |
| 3 | BC | 55 | ILE | 5.0 |
| 31 | CK | 3 | THR | 5.0 |
| 22 | CA | 1876 | A | 5.0 |
| 45 | CY | 46 | PHE | 5.0 |
| 19 | AS | 23 | VAL | 5.0 |
| 26 | CE | 167 | VAL | 5.0 |
| 28 | CG | 94 | TYR | 5.0 |
| 40 | CT | 49 | LYS | 5.0 |
| 3 | BC | 148 | GLY | 5.0 |
| 22 | CA | 884 | U | 5.0 |
| 2 | BB | 6 | MET | 5.0 |
| 10 | BJ | 61 | ALA | 5.0 |
| 13 | AM | 35 | ALA | 5.0 |
| 25 | CD | 41 | ALA | 5.0 |
| 26 | CE | 148 | ILE | 5.0 |
| 49 | C2 | 32 | GLU | 5.0 |
| 14 | BN | 95 | GLY | 5.0 |
| 41 | CU | 90 | GLY | 5.0 |
| 46 | CZ | 42 | LEU | 5.0 |
| 24 | CC | 112 | ALA | 5.0 |
| 9 | BI | 91 | ASP | 5.0 |
| 22 | CA | 12 | U | 5.0 |
| 26 | CE | 73 | ILE | 5.0 |
| 19 | BS | 72 | GLY | 5.0 |
| 1 | AA | 844 | G | 5.0 |
| 22 | CA | 273 | G | 5.0 |
| 26 | CE | 113 | VAL | 5.0 |
| 26 | CE | 186 | VAL | 5.0 |
| 40 | CT | 16 | LYS | 5.0 |
| 1 | AA | 91 | U | 5.0 |
| 1 | BA | 1028 | C | 5.0 |
| 5 | BE | 103 | THR | 5.0 |
| 7 | BG | 143 | ARG | 5.0 |
| 13 | BM | 92 | ARG | 5.0 |
| 16 | BP | 56 | ARG | 5.0 |
| 17 | BQ | 51 | ASN | 5.0 |
| 27 | CF | 67 | ILE | 5.0 |
| 13 | BM | 78 | LYS | 5.0 |
| 22 | CA | 1082 | U | 5.0 |
| 28 | CG | 6 | LYS | 5.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 55 | DI | 115 | GLY | 5.0 |
| 2 | BB | 184 | PHE | 5.0 |
| 1 | AA | 90 | C | 5.0 |
| 9 | BI | 32 | GLN | 5.0 |
| 22 | CA | 178 | G | 5.0 |
| 1 | BA | 190 | A | 5.0 |
| 7 | AG | 79 | ARG | 5.0 |
| 7 | BG | 70 | ARG | 5.0 |
| 8 | AH | 54 | ASP | 5.0 |
| 14 | BN | 81 | ARG | 5.0 |
| 22 | CA | 1872 | A | 5.0 |
| 23 | CB | 57 | A | 5.0 |
| 25 | CD | 180 | VAL | 5.0 |
| 30 | CJ | 125 | MET | 5.0 |
| 14 | AN | 22 | ALA | 5.0 |
| 33 | CM | 98 | ALA | 5.0 |
| 33 | CM | 129 | LYS | 4.9 |
| 29 | DH | 16 | GLY | 4.9 |
| 33 | CM | 135 | ILE | 4.9 |
| 7 | BG | 9 | GLN | 4.9 |
| 42 | CV | 18 | ASP | 4.9 |
| 22 | CA | 136 | G | 4.9 |
| 53 | DA | 1068 | G | 4.9 |
| 1 | BA | 1330 | U | 4.9 |
| 22 | CA | 546 | U | 4.9 |
| 26 | CE | 18 | THR | 4.9 |
| 29 | CH | 65 | ALA | 4.9 |
| 37 | DQ | 115 | ASN | 4.9 |
| 44 | CX | 38 | VAL | 4.9 |
| 2 | AB | 62 | SER | 4.9 |
| 1 | BA | 84 | U | 4.9 |
| 1 | BA | 1133 | G | 4.9 |
| 35 | CO | 74 | GLU | 4.9 |
| 8 | AH | 24 | ALA | 4.9 |
| 15 | BO | 79 | THR | 4.9 |
| 20 | AT | 46 | ALA | 4.9 |
| 42 | CV | 3 | ALA | 4.9 |
| 49 | C2 | 23 | THR | 4.9 |
| 2 | BB | 107 | VAL | 4.9 |
| 2 | BB | 187 | VAL | 4.9 |
| 3 | AC | 41 | GLN | 4.9 |
| 4 | BD | 44 | ARG | 4.9 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 14 | BN | 61 | ARG | 4.9 |
| 1 | BA | 1011 | C | 4.9 |
| 1 | BA | 1267 | C | 4.9 |
| 22 | CA | 140 | C | 4.9 |
| 28 | CG | 21 | GLY | 4.9 |
| 30 | CJ | 116 | ASP | 4.9 |
| 41 | CU | 14 | PRO | 4.9 |
| 1 | BA | 1248 | A | 4.9 |
| 7 | AG | 42 | ILE | 4.9 |
| 53 | DA | 882 | G | 4.9 |
| 36 | CP | 7 | ARG | 4.9 |
| 50 | C3 | 12 | ARG | 4.9 |
| 7 | BG | 39 | ALA | 4.9 |
| 21 | BU | 57 | ALA | 4.9 |
| 29 | DH | 84 | ALA | 4.9 |
| 26 | CE | 7 | ASP | 4.9 |
| 30 | DJ | 64 | ASP | 4.9 |
| 17 | BQ | 23 | VAL | 4.9 |
| 28 | CG | 43 | VAL | 4.9 |
| 31 | CK | 139 | VAL | 4.9 |
| 42 | CV | 42 | VAL | 4.9 |
| 44 | CX | 70 | GLU | 4.9 |
| 47 | C0 | 26 | GLY | 4.9 |
| 55 | DI | 116 | GLU | 4.9 |
| 1 | BA | 205 | A | 4.9 |
| 22 | CA | 1054 | A | 4.9 |
| 25 | CD | 40 | LEU | 4.9 |
| 45 | CY | 71 | LEU | 4.9 |
| 22 | CA | 137 | U | 4.9 |
| 3 | BC | 41 | GLN | 4.9 |
| 1 | BA | 988 | G | 4.9 |
| 1 | BA | 1309 | G | 4.9 |
| 1 | BA | 1316 | G | 4.9 |
| 22 | CA | 88 | G | 4.9 |
| 7 | BG | 7 | ILE | 4.9 |
| 51 | C4 | 59 | ILE | 4.9 |
| 52 | C5 | 16 | ILE | 4.9 |
| 11 | BK | 75 | LYS | 4.9 |
| 6 | BF | 76 | THR | 4.9 |
| 24 | CC | 31 | ALA | 4.9 |
| 48 | C1 | 23 | THR | 4.9 |
| 7 | AG | 82 | GLY | 4.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | BC | 203 | PHE | 4.9 |
| 2 | AB | 187 | VAL | 4.9 |
| 43 | CW | 8 | VAL | 4.9 |
| 14 | BN | 79 | LEU | 4.9 |
| 18 | AR | 32 | TYR | 4.9 |
| 45 | CY | 78 | TYR | 4.9 |
| 29 | DH | 149 | GLU | 4.9 |
| 1 | BA | 1001 | C | 4.9 |
| 3 | BC | 31 | ASP | 4.9 |
| 13 | AM | 115 | PRO | 4.9 |
| 14 | BN | 50 | THR | 4.9 |
| 29 | CH | 52 | ALA | 4.9 |
| 34 | CN | 37 | GLY | 4.9 |
| 34 | CN | 56 | ALA | 4.9 |
| 15 | BO | 83 | GLU | 4.8 |
| 30 | CJ | 81 | LYS | 4.8 |
| 20 | AT | 66 | LEU | 4.8 |
| 22 | CA | 2127 | G | 4.8 |
| 22 | CA | 2660 | A | 4.8 |
| 24 | CC | 29 | PRO | 4.8 |
| 20 | BT | 64 | LYS | 4.8 |
| 28 | CG | 99 | LYS | 4.8 |
| 28 | CG | 136 | ALA | 4.8 |
| 30 | DJ | 63 | ALA | 4.8 |
| 33 | CM | 132 | ARG | 4.8 |
| 36 | CP | 37 | ALA | 4.8 |
| 41 | DU | 52 | GLU | 4.8 |
| 44 | CX | 82 | ILE | 4.8 |
| 1 | BA | 1136 | C | 4.8 |
| 7 | AG | 64 | VAL | 4.8 |
| 9 | AI | 48 | VAL | 4.8 |
| 2 | AB | 141 | LEU | 4.8 |
| 15 | BO | 32 | LEU | 4.8 |
| 29 | CH | 54 | LEU | 4.8 |
| 9 | BI | 82 | GLY | 4.8 |
| 22 | CA | 1085 | A | 4.8 |
| 33 | CM | 143 | GLU | 4.8 |
| 26 | CE | 40 | ARG | 4.8 |
| 44 | CX | 54 | GLY | 4.8 |
| 3 | BC | 30 | ALA | 4.8 |
| 6 | AF | 105 | ALA | 4.8 |
| 11 | AK | 103 | ALA | 4.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | CA | 1539 | U | 4.8 |
| 14 | AN | 31 | ILE | 4.8 |
| 1 | BA | 1452 | C | 4.8 |
| 14 | AN | 23 | LYS | 4.8 |
| 39 | CS | 54 | VAL | 4.8 |
| 3 | AC | 81 | GLY | 4.8 |
| 13 | AM | 8 | ASN | 4.8 |
| 13 | BM | 111 | GLY | 4.8 |
| 30 | DJ | 25 | GLY | 4.8 |
| 55 | DI | 16 | SER | 4.8 |
| 2 | BB | 125 | THR | 4.8 |
| 13 | AM | 32 | ALA | 4.8 |
| 55 | DI | 83 | ALA | 4.8 |
| 3 | BC | 94 | ILE | 4.8 |
| 49 | D2 | 53 | LYS | 4.8 |
| 46 | CZ | 47 | ARG | 4.8 |
| 41 | CU | 24 | MET | 4.8 |
| 13 | AM | 16 | VAL | 4.8 |
| 2 | AB | 85 | LEU | 4.8 |
| 22 | CA | 1529 | G | 4.8 |
| 36 | CP | 2 | ASP | 4.8 |
| 52 | C5 | 10 | LEU | 4.8 |
| 20 | BT | 63 | ALA | 4.8 |
| 29 | CH | 81 | ALA | 4.8 |
| 43 | CW | 54 | ALA | 4.8 |
| 34 | CN | 55 | ARG | 4.8 |
| 1 | BA | 1254 | A | 4.8 |
| 1 | BA | 1340 | A | 4.8 |
| 22 | CA | 2171 | A | 4.8 |
| 2 | AB | 77 | SER | 4.8 |
| 7 | AG | 81 | GLY | 4.8 |
| 2 | BB | 127 | ASP | 4.8 |
| 9 | AI | 89 | GLU | 4.8 |
| 39 | CS | 34 | GLU | 4.8 |
| 2 | AB | 69 | PHE | 4.8 |
| 10 | AJ | 74 | VAL | 4.8 |
| 29 | DH | 78 | VAL | 4.8 |
| 43 | CW | 64 | VAL | 4.8 |
| 20 | BT | 72 | ALA | 4.8 |
| 13 | BM | 105 | ASN | 4.8 |
| 3 | BC | 147 | LYS | 4.8 |
| 1 | AA | 85 | U | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | CH | 38 | PRO | 4.7 |
| 22 | CA | 1452 | G | 4.7 |
| 9 | BI | 113 | ARG | 4.7 |
| 29 | DH | 97 | ARG | 4.7 |
| 9 | BI | 87 | LEU | 4.7 |
| 15 | BO | 67 | LEU | 4.7 |
| 44 | CX | 71 | VAL | 4.7 |
| 6 | AF | 32 | ALA | 4.7 |
| 25 | CD | 85 | ALA | 4.7 |
| 22 | CA | 272 | A | 4.7 |
| 22 | CA | 892 | A | 4.7 |
| 51 | C4 | 64 | TYR | 4.7 |
| 13 | AM | 85 | CYS | 4.7 |
| 8 | BH | 44 | GLY | 4.7 |
| 36 | CP | 34 | HIS | 4.7 |
| 2 | BB | 151 | ILE | 4.7 |
| 7 | AG | 7 | ILE | 4.7 |
| 22 | CA | 289 | G | 4.7 |
| 3 | BC | 79 | LYS | 4.7 |
| 14 | BN | 83 | LYS | 4.7 |
| 1 | AA | 1035 | A | 4.7 |
| 22 | CA | 2309 | A | 4.7 |
| 37 | CQ | 30 | VAL | 4.7 |
| 41 | CU | 7 | LEU | 4.7 |
| 50 | C3 | 5 | PHE | 4.7 |
| 51 | C4 | 29 | LEU | 4.7 |
| 2 | AB | 55 | ALA | 4.7 |
| 7 | AG | 8 | GLY | 4.7 |
| 28 | CG | 120 | GLY | 4.7 |
| 33 | CM | 16 | GLY | 4.7 |
| 27 | DF | 80 | ARG | 4.7 |
| 14 | BN | 70 | PRO | 4.7 |
| 17 | AQ | 5 | ILE | 4.7 |
| 22 | CA | 2110 | G | 4.7 |
| 53 | DA | 2136 | G | 4.7 |
| 14 | BN | 67 | THR | 4.7 |
| 22 | CA | 2163 | A | 4.7 |
| 6 | BF | 8 | PHE | 4.7 |
| 13 | BM | 100 | GLN | 4.7 |
| 43 | CW | 61 | LEU | 4.7 |
| 44 | CX | 77 | ARG | 4.7 |
| 45 | CY | 30 | LEU | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 17 | BQ | 54 | GLY | 4.7 |
| 19 | BS | 20 | GLU | 4.7 |
| 26 | CE | 35 | TYR | 4.7 |
| 1 | BA | 1242 | G | 4.7 |
| 22 | CA | 1861 | G | 4.7 |
| 23 | CB | 58 | A | 4.7 |
| 1 | BA | 1296 | C | 4.7 |
| 1 | BA | 1029 | U | 4.7 |
| 9 | BI | 122 | ARG | 4.7 |
| 22 | CA | 1108 | U | 4.7 |
| 36 | CP | 84 | GLU | 4.7 |
| 49 | C2 | 17 | THR | 4.7 |
| 10 | BJ | 15 | HIS | 4.7 |
| 21 | AU | 5 | LYS | 4.7 |
| 55 | DI | 111 | ALA | 4.7 |
| 14 | AN | 42 | TRP | 4.7 |
| 26 | CE | 180 | LEU | 4.7 |
| 40 | CT | 69 | LEU | 4.7 |
| 5 | BE | 70 | ASN | 4.7 |
| 7 | BG | 63 | GLU | 4.7 |
| 22 | CA | 1073 | A | 4.7 |
| 22 | CA | 1583 | A | 4.7 |
| 50 | C3 | 6 | GLN | 4.7 |
| 14 | BN | 47 | LYS | 4.7 |
| 55 | DI | 86 | THR | 4.7 |
| 29 | DH | 136 | SER | 4.7 |
| 40 | CT | 13 | SER | 4.7 |
| 2 | AB | 68 | LEU | 4.7 |
| 9 | BI | 35 | LEU | 4.7 |
| 10 | AJ | 49 | PHE | 4.7 |
| 3 | BC | 131 | ARG | 4.7 |
| 3 | BC | 132 | ARG | 4.7 |
| 12 | BL | 14 | ARG | 4.7 |
| 36 | CP | 16 | ARG | 4.7 |
| 2 | AB | 224 | GLY | 4.6 |
| 15 | BO | 33 | THR | 4.6 |
| 31 | CK | 142 | ILE | 4.6 |
| 32 | CL | 2 | ILE | 4.6 |
| 27 | CF | 71 | ARG | 4.6 |
| 7 | BG | 47 | LEU | 4.6 |
| 24 | CC | 67 | PHE | 4.6 |
| 25 | CD | 101 | PHE | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | CA | 287 | G | 4.6 |
| 8 | AH | 65 | TYR | 4.6 |
| 28 | CG | 127 | THR | 4.6 |
| 41 | CU | 21 | SER | 4.6 |
| 45 | CY | 8 | THR | 4.6 |
| 27 | CF | 125 | ARG | 4.6 |
| 3 | BC | 207 | ILE | 4.6 |
| 29 | CH | 78 | VAL | 4.6 |
| 30 | DJ | 57 | VAL | 4.6 |
| 39 | CS | 75 | VAL | 4.6 |
| 35 | CO | 80 | PHE | 4.6 |
| 2 | AB | 132 | LYS | 4.6 |
| 22 | CA | 93 | G | 4.6 |
| 27 | CF | 62 | GLY | 4.6 |
| 34 | CN | 106 | ASP | 4.6 |
| 46 | CZ | 9 | LYS | 4.6 |
| 3 | BC | 164 | ARG | 4.6 |
| 41 | CU | 29 | THR | 4.6 |
| 22 | CA | 1748 | C | 4.6 |
| 22 | CA | 1874 | C | 4.6 |
| 23 | CB | 19 | C | 4.6 |
| 2 | AB | 34 | ALA | 4.6 |
| 20 | BT | 22 | ALA | 4.6 |
| 27 | CF | 53 | ALA | 4.6 |
| 2 | AB | 67 | ILE | 4.6 |
| 2 | AB | 164 | ILE | 4.6 |
| 7 | AG | 21 | GLU | 4.6 |
| 9 | BI | 79 | ILE | 4.6 |
| 28 | CG | 26 | ILE | 4.6 |
| 33 | CM | 115 | GLU | 4.6 |
| 28 | CG | 18 | LYS | 4.6 |
| 2 | BB | 199 | VAL | 4.6 |
| 25 | CD | 20 | VAL | 4.6 |
| 25 | CD | 201 | LEU | 4.6 |
| 46 | CZ | 49 | ASP | 4.6 |
| 50 | C3 | 31 | LEU | 4.6 |
| 3 | AC | 126 | ARG | 4.6 |
| 7 | BG | 82 | GLY | 4.6 |
| 29 | DH | 47 | PHE | 4.6 |
| 2 | AB | 84 | ALA | 4.6 |
| 2 | BB | 55 | ALA | 4.6 |
| 2 | BB | 75 | ALA | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | CH | 67 | ALA | 4.6 |
| 45 | DY | 77 | LYS | 4.6 |
| 10 | BJ | 7 | ARG | 4.6 |
| 14 | BN | 9 | ARG | 4.6 |
| 28 | CG | 35 | ARG | 4.6 |
| 30 | CJ | 107 | GLN | 4.6 |
| 7 | AG | 19 | GLY | 4.6 |
| 11 | AK | 19 | GLY | 4.6 |
| 41 | CU | 78 | SER | 4.6 |
| 22 | CA | 329 | G | 4.6 |
| 29 | CH | 19 | VAL | 4.6 |
| 46 | CZ | 17 | GLU | 4.6 |
| 37 | CQ | 60 | THR | 4.6 |
| 42 | CV | 55 | PRO | 4.6 |
| 2 | BB | 108 | ARG | 4.6 |
| 41 | CU | 3 | ARG | 4.6 |
| 1 | BA | 212 | G | 4.6 |
| 1 | BA | 1252 | A | 4.6 |
| 7 | AG | 23 | LEU | 4.6 |
| 22 | CA | 1459 | G | 4.6 |
| 22 | CA | 2322 | A | 4.6 |
| 23 | CB | 119 | A | 4.6 |
| 53 | DA | 548 | G | 4.6 |
| 55 | DI | 59 | LEU | 4.6 |
| 6 | BF | 96 | VAL | 4.6 |
| 7 | AG | 69 | VAL | 4.6 |
| 26 | DE | 4 | VAL | 4.6 |
| 29 | CH | 79 | THR | 4.5 |
| 29 | CH | 97 | ARG | 4.5 |
| 50 | C3 | 35 | ARG | 4.5 |
| 17 | BQ | 57 | ASP | 4.5 |
| 33 | CM | 104 | GLN | 4.5 |
| 9 | BI | 36 | GLU | 4.5 |
| 48 | C1 | 21 | ALA | 4.5 |
| 53 | DA | 2104 | C | 4.5 |
| 3 | BC | 155 | GLY | 4.5 |
| 41 | CU | 26 | LYS | 4.5 |
| 53 | DA | 2180 | U | 4.5 |
| 22 | CA | 259 | G | 4.5 |
| 37 | CQ | 110 | ILE | 4.5 |
| 38 | CR | 8 | VAL | 4.5 |
| 2 | AB | 45 | LYS | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | BF | 93 | LYS | 4.5 |
| 33 | CM | 1 | MET | 4.5 |
| 39 | CS | 1 | MET | 4.5 |
| 7 | BG | 139 | GLU | 4.5 |
| 9 | AI | 50 | GLN | 4.5 |
| 1 | BA | 1222 | G | 4.5 |
| 22 | CA | 2123 | G | 4.5 |
| 7 | BG | 29 | ILE | 4.5 |
| 41 | CU | 64 | LYS | 4.5 |
| 55 | DI | 68 | PRO | 4.5 |
| 1 | AA | 1132 | C | 4.5 |
| 2 | BB | 166 | ALA | 4.5 |
| 6 | BF | 28 | ALA | 4.5 |
| 15 | BO | 76 | ALA | 4.5 |
| 31 | CK | 79 | GLY | 4.5 |
| 50 | C3 | 18 | PHE | 4.5 |
| 54 | DD | 132 | ALA | 4.5 |
| 3 | BC | 110 | GLU | 4.5 |
| 15 | AO | 89 | ARG | 4.5 |
| 31 | CK | 96 | ARG | 4.5 |
| 3 | AC | 42 | TYR | 4.5 |
| 17 | BQ | 16 | LYS | 4.5 |
| 1 | BA | 1278 | G | 4.5 |
| 22 | CA | 1743 | G | 4.5 |
| 53 | DA | 1731 | G | 4.5 |
| 3 | BC | 32 | ASN | 4.5 |
| 19 | AS | 47 | LEU | 4.5 |
| 28 | CG | 37 | LEU | 4.5 |
| 40 | CT | 33 | LEU | 4.5 |
| 5 | BE | 120 | VAL | 4.5 |
| 13 | AM | 43 | VAL | 4.5 |
| 16 | BP | 20 | VAL | 4.5 |
| 26 | CE | 193 | VAL | 4.5 |
| 49 | C2 | 12 | VAL | 4.5 |
| 50 | C3 | 9 | VAL | 4.5 |
| 3 | BC | 129 | MET | 4.5 |
| 1 | AA | 1036 | A | 4.5 |
| 22 | CA | 895 | U | 4.5 |
| 25 | CD | 11 | MET | 4.5 |
| 28 | CG | 64 | GLN | 4.5 |
| 38 | CR | 113 | ALA | 4.5 |
| 26 | CE | 23 | PHE | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 11 | BK | 70 | CYS | 4.5 |
| 9 | BI | 124 | ARG | 4.5 |
| 22 | CA | 1534 | U | 4.5 |
| 2 | AB | 11 | LYS | 4.5 |
| 3 | BC | 64 | ILE | 4.5 |
| 20 | BT | 42 | GLY | 4.5 |
| 21 | BU | 27 | GLY | 4.5 |
| 27 | CF | 41 | GLY | 4.5 |
| 29 | CH | 80 | ILE | 4.5 |
| 30 | DJ | 111 | GLN | 4.5 |
| 31 | CK | 54 | ILE | 4.5 |
| 1 | BA | 1042 | A | 4.5 |
| 8 | BH | 130 | ALA | 4.5 |
| 15 | BO | 12 | VAL | 4.5 |
| 17 | BQ | 29 | VAL | 4.5 |
| 29 | DH | 69 | ALA | 4.5 |
| 1 | BA | 984 | C | 4.5 |
| 22 | CA | 343 | C | 4.5 |
| 23 | CB | 30 | C | 4.5 |
| 13 | BM | 14 | HIS | 4.5 |
| 22 | CA | 2181 | U | 4.5 |
| 10 | AJ | 5 | ARG | 4.5 |
| 20 | BT | 56 | PRO | 4.5 |
| 35 | CO | 2 | ARG | 4.5 |
| 50 | C3 | 25 | LYS | 4.5 |
| 2 | BB | 8 | ASP | 4.5 |
| 9 | AI | 82 | GLY | 4.5 |
| 15 | AO | 16 | GLY | 4.5 |
| 22 | CA | 144 | A | 4.5 |
| 26 | CE | 80 | SER | 4.5 |
| 53 | DA | 613 | A | 4.5 |
| 2 | BB | 60 | ILE | 4.4 |
| 45 | CY | 49 | LEU | 4.4 |
| 11 | BK | 21 | ALA | 4.4 |
| 20 | AT | 62 | ALA | 4.4 |
| 21 | BU | 7 | ARG | 4.4 |
| 44 | CX | 78 | LYS | 4.4 |
| 1 | BA | 1043 | G | 4.4 |
| 29 | DH | 17 | ASP | 4.4 |
| 41 | CU | 22 | THR | 4.4 |
| 1 | BA | 1308 | U | 4.4 |
| 41 | CU | 54 | GLU | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | BA | 1327 | C | 4.4 |
| 22 | CA | 145 | C | 4.4 |
| 22 | CA | 1043 | C | 4.4 |
| 3 | BC | 8 | ASN | 4.4 |
| 29 | DH | 73 | ASN | 4.4 |
| 6 | BF | 29 | ILE | 4.4 |
| 10 | AJ | 102 | LEU | 4.4 |
| 40 | CT | 19 | LEU | 4.4 |
| 2 | BB | 221 | VAL | 4.4 |
| 28 | CG | 23 | VAL | 4.4 |
| 42 | CV | 45 | HIS | 4.4 |
| 52 | C5 | 22 | VAL | 4.4 |
| 54 | DD | 142 | VAL | 4.4 |
| 22 | CA | 180 | G | 4.4 |
| 22 | CA | 1063 | G | 4.4 |
| 27 | CF | 124 | GLY | 4.4 |
| 55 | DI | 90 | GLY | 4.4 |
| 19 | AS | 21 | LYS | 4.4 |
| 22 | CA | 268 | C | 4.4 |
| 22 | CA | 1064 | C | 4.4 |
| 13 | BM | 98 | ARG | 4.4 |
| 40 | CT | 31 | GLN | 4.4 |
| 21 | BU | 56 | HIS | 4.4 |
| 28 | CG | 96 | ALA | 4.4 |
| 31 | CK | 94 | ALA | 4.4 |
| 22 | CA | 2166 | U | 4.4 |
| 11 | AK | 86 | VAL | 4.4 |
| 29 | CH | 110 | VAL | 4.4 |
| 39 | CS | 72 | VAL | 4.4 |
| 45 | CY | 13 | VAL | 4.4 |
| 1 | AA | 81 | A | 4.4 |
| 2 | AB | 131 | LYS | 4.4 |
| 33 | CM | 84 | LYS | 4.4 |
| 45 | CY | 55 | GLY | 4.4 |
| 22 | CA | 1728 | C | 4.4 |
| 28 | CG | 110 | SER | 4.4 |
| 28 | CG | 3 | ARG | 4.4 |
| 22 | CA | 2797 | U | 4.4 |
| 16 | BP | 48 | GLU | 4.4 |
| 19 | AS | 14 | HIS | 4.4 |
| 3 | BC | 111 | LEU | 4.4 |
| 11 | AK | 23 | ILE | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | CA | 1103 | A | 4.4 |
| 22 | CA | 2147 | A | 4.4 |
| 24 | CC | 74 | ILE | 4.4 |
| 8 | BH | 127 | CYS | 4.4 |
| 23 | CB | 35 | C | 4.4 |
| 26 | CE | 42 | GLY | 4.4 |
| 26 | CE | 83 | VAL | 4.4 |
| 26 | CE | 102 | ARG | 4.4 |
| 22 | CA | 548 | G | 4.4 |
| 22 | CA | 1106 | G | 4.4 |
| 23 | CB | 54 | G | 4.4 |
| 41 | CU | 27 | SER | 4.4 |
| 2 | BB | 142 | GLU | 4.4 |
| 28 | CG | 124 | GLU | 4.4 |
| 43 | CW | 91 | PHE | 4.4 |
| 14 | BN | 54 | ASP | 4.4 |
| 29 | CH | 106 | ALA | 4.4 |
| 31 | CK | 75 | TYR | 4.4 |
| 48 | D1 | 2 | ALA | 4.4 |
| 49 | C2 | 15 | ALA | 4.4 |
| 9 | BI | 117 | GLY | 4.4 |
| 22 | CA | 143 | C | 4.4 |
| 25 | CD | 72 | GLY | 4.4 |
| 30 | CJ | 91 | GLY | 4.4 |
| 3 | BC | 119 | SER | 4.4 |
| 20 | BT | 78 | ASN | 4.4 |
| 39 | CS | 87 | GLN | 4.4 |
| 36 | CP | 45 | SER | 4.4 |
| 9 | AI | 67 | VAL | 4.4 |
| 22 | CA | 2102 | G | 4.4 |
| 6 | AF | 104 | LYS | 4.4 |
| 1 | BA | 1264 | U | 4.4 |
| 2 | BB | 158 | PRO | 4.3 |
| 29 | DH | 133 | GLN | 4.3 |
| 34 | CN | 111 | GLU | 4.3 |
| 38 | CR | 116 | ALA | 4.3 |
| 13 | BM | 88 | GLY | 4.3 |
| 30 | CJ | 19 | ASN | 4.3 |
| 2 | BB | 214 | LEU | 4.3 |
| 3 | BC | 204 | LYS | 4.3 |
| 1 | BA | 973 | G | 4.3 |
| 28 | CG | 47 | ASP | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | CA | 1729 | U | 4.3 |
| 34 | CN | 96 | ILE | 4.3 |
| 54 | DD | 146 | ILE | 4.3 |
| 25 | CD | 9 | VAL | 4.3 |
| 33 | CM | 118 | THR | 4.3 |
| 37 | CQ | 9 | GLU | 4.3 |
| 40 | CT | 59 | GLU | 4.3 |
| 44 | CX | 85 | GLU | 4.3 |
| 2 | BB | 182 | PRO | 4.3 |
| 10 | BJ | 43 | PRO | 4.3 |
| 54 | DD | 143 | PRO | 4.3 |
| 5 | BE | 53 | ALA | 4.3 |
| 12 | BL | 123 | LYS | 4.3 |
| 16 | BP | 58 | ALA | 4.3 |
| 25 | CD | 87 | GLY | 4.3 |
| 29 | DH | 85 | GLY | 4.3 |
| 32 | CL | 16 | ALA | 4.3 |
| 33 | CM | 134 | ALA | 4.3 |
| 26 | CE | 168 | ASP | 4.3 |
| 48 | C1 | 18 | SER | 4.3 |
| 32 | CL | 32 | TYR | 4.3 |
| 9 | AI | 52 | LEU | 4.3 |
| 22 | CA | 1177 | G | 4.3 |
| 22 | CA | 1530 | G | 4.3 |
| 48 | C1 | 52 | ARG | 4.3 |
| 23 | CB | 114 | C | 4.3 |
| 1 | AA | 1000 | A | 4.3 |
| 1 | AA | 1004 | A | 4.3 |
| 1 | AA | 1019 | A | 4.3 |
| 1 | BA | 461 | A | 4.3 |
| 34 | CN | 101 | VAL | 4.3 |
| 40 | CT | 50 | VAL | 4.3 |
| 27 | CF | 3 | LYS | 4.3 |
| 28 | CG | 29 | LYS | 4.3 |
| 28 | CG | 126 | PRO | 4.3 |
| 29 | DH | 118 | PRO | 4.3 |
| 55 | DI | 74 | ASP | 4.3 |
| 1 | BA | 1017 | U | 4.3 |
| 3 | AC | 80 | LYS | 4.3 |
| 9 | BI | 114 | LYS | 4.3 |
| 49 | C2 | 50 | LYS | 4.3 |
| 25 | CD | 60 | VAL | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | CH | 51 | ARG | 4.3 |
| 45 | CY | 29 | PHE | 4.3 |
| 11 | AK | 80 | LYS | 4.3 |
| 22 | CA | 2585 | U | 4.3 |
| 29 | CH | 41 | LYS | 4.3 |
| 1 | BA | 1294 | G | 4.3 |
| 1 | BA | 1305 | G | 4.3 |
| 5 | BE | 80 | THR | 4.3 |
| 40 | CT | 100 | THR | 4.3 |
| 18 | BR | 51 | TYR | 4.3 |
| 31 | CK | 16 | TYR | 4.3 |
| 2 | AB | 44 | GLU | 4.3 |
| 28 | CG | 75 | MET | 4.3 |
| 45 | CY | 56 | MET | 4.3 |
| 28 | CG | 8 | PRO | 4.3 |
| 46 | CZ | 35 | GLY | 4.3 |
| 16 | BP | 4 | ILE | 4.3 |
| 16 | BP | 57 | ILE | 4.3 |
| 42 | CV | 103 | ILE | 4.3 |
| 2 | AB | 217 | VAL | 4.3 |
| 6 | AF | 96 | VAL | 4.3 |
| 50 | C3 | 14 | ARG | 4.3 |
| 1 | BA | 1009 | U | 4.3 |
| 2 | BB | 89 | GLN | 4.3 |
| 43 | CW | 51 | GLN | 4.3 |
| 11 | AK | 41 | ALA | 4.3 |
| 13 | AM | 40 | ALA | 4.3 |
| 19 | AS | 39 | THR | 4.3 |
| 29 | DH | 86 | ASP | 4.3 |
| 10 | BJ | 48 | ARG | 4.3 |
| 33 | CM | 69 | ARG | 4.3 |
| 13 | BM | 115 | PRO | 4.3 |
| 37 | CQ | 98 | TYR | 4.3 |
| 30 | CJ | 102 | SER | 4.3 |
| 30 | CJ | 105 | GLN | 4.3 |
| 17 | BQ | 58 | VAL | 4.3 |
| 9 | BI | 108 | ALA | 4.3 |
| 13 | BM | 72 | GLU | 4.3 |
| 43 | CW | 35 | GLU | 4.3 |
| 53 | DA | 2171 | A | 4.2 |
| 22 | CA | 2172 | U | 4.2 |
| 24 | CC | 30 | PHE | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 28 | CG | 16 | ASP | 4.2 |
| 39 | CS | 55 | ASP | 4.2 |
| 40 | CT | 34 | ASP | 4.2 |
| 43 | CW | 2 | PHE | 4.2 |
| 21 | AU | 21 | ARG | 4.2 |
| 30 | DJ | 119 | GLY | 4.2 |
| 41 | DU | 91 | GLN | 4.2 |
| 41 | CU | 42 | GLU | 4.2 |
| 53 | DA | 2170 | A | 4.2 |
| 12 | BL | 60 | GLY | 4.2 |
| 25 | CD | 19 | GLY | 4.2 |
| 26 | CE | 56 | GLY | 4.2 |
| 28 | CG | 108 | GLY | 4.2 |
| 37 | CQ | 59 | PHE | 4.2 |
| 39 | CS | 45 | GLU | 4.2 |
| 53 | DA | 893 | C | 4.2 |
| 13 | AM | 80 | LEU | 4.2 |
| 14 | AN | 33 | ASP | 4.2 |
| 24 | CC | 28 | LYS | 4.2 |
| 26 | CE | 156 | ASN | 4.2 |
| 28 | CG | 133 | LEU | 4.2 |
| 32 | CL | 108 | ARG | 4.2 |
| 38 | CR | 11 | ARG | 4.2 |
| 21 | AU | 50 | ALA | 4.2 |
| 28 | CG | 63 | ALA | 4.2 |
| 32 | CL | 60 | ALA | 4.2 |
| 43 | CW | 74 | ALA | 4.2 |
| 36 | CP | 27 | VAL | 4.2 |
| 45 | CY | 58 | VAL | 4.2 |
| 25 | CD | 30 | GLU | 4.2 |
| 27 | CF | 101 | GLU | 4.2 |
| 13 | AM | 20 | THR | 4.2 |
| 22 | CA | 1531 | C | 4.2 |
| 22 | CA | 1546 | G | 4.2 |
| 54 | DD | 161 | MET | 4.2 |
| 7 | AG | 149 | LYS | 4.2 |
| 9 | BI | 103 | PHE | 4.2 |
| 48 | C1 | 32 | LYS | 4.2 |
| 29 | DH | 128 | HIS | 4.2 |
| 18 | BR | 67 | LEU | 4.2 |
| 26 | CE | 25 | GLU | 4.2 |
| 48 | C1 | 22 | LEU | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 7 | BG | 127 | ALA | 4.2 |
| 39 | DS | 103 | ALA | 4.2 |
| 9 | BI | 19 | VAL | 4.2 |
| 22 | CA | 2165 | C | 4.2 |
| 24 | CC | 3 | VAL | 4.2 |
| 24 | CC | 56 | GLY | 4.2 |
| 37 | CQ | 33 | VAL | 4.2 |
| 3 | BC | 38 | LYS | 4.2 |
| 22 | CA | 1724 | G | 4.2 |
| 22 | CA | 1875 | G | 4.2 |
| 3 | BC | 140 | ASN | 4.2 |
| 11 | BK | 15 | GLN | 4.2 |
| 5 | AE | 115 | LEU | 4.2 |
| 22 | CA | 2129 | C | 4.2 |
| 36 | CP | 26 | LEU | 4.2 |
| 38 | CR | 99 | ALA | 4.2 |
| 55 | DI | 25 | ALA | 4.2 |
| 2 | BB | 38 | VAL | 4.2 |
| 29 | CH | 149 | GLU | 4.2 |
| 49 | C2 | 24 | THR | 4.2 |
| 53 | DA | 285 | G | 4.2 |
| 55 | DI | 99 | PHE | 4.2 |
| 6 | BF | 34 | GLY | 4.2 |
| 25 | CD | 115 | GLY | 4.2 |
| 26 | CE | 36 | ALA | 4.2 |
| 29 | CH | 126 | GLY | 4.2 |
| 37 | CQ | 108 | ALA | 4.2 |
| 1 | BA | 844 | G | 4.1 |
| 3 | BC | 70 | THR | 4.1 |
| 10 | BJ | 83 | THR | 4.1 |
| 29 | CH | 21 | VAL | 4.1 |
| 29 | CH | 61 | VAL | 4.1 |
| 51 | D4 | 7 | VAL | 4.1 |
| 21 | AU | 25 | LYS | 4.1 |
| 22 | CA | 1065 | U | 4.1 |
| 22 | CA | 2793 | C | 4.1 |
| 7 | AG | 4 | ARG | 4.1 |
| 5 | BE | 158 | GLY | 4.1 |
| 28 | CG | 31 | GLY | 4.1 |
| 11 | AK | 102 | ALA | 4.1 |
| 28 | CG | 5 | ALA | 4.1 |
| 47 | D0 | 2[A] | ALA | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | BB | 114 | LEU | 4.1 |
| 1 | BA | 81 | A | 4.1 |
| 1 | BA | 1275 | A | 4.1 |
| 20 | BT | 16 | LYS | 4.1 |
| 22 | CA | 1532 | A | 4.1 |
| 24 | CC | 111 | LYS | 4.1 |
| 24 | CC | 265 | LYS | 4.1 |
| 1 | AA | 1134 | G | 4.1 |
| 2 | AB | 9 | MET | 4.1 |
| 22 | CA | 308 | G | 4.1 |
| 22 | CA | 2186 | G | 4.1 |
| 1 | BA | 632 | U | 4.1 |
| 22 | CA | 1101 | U | 4.1 |
| 33 | CM | 67 | THR | 4.1 |
| 36 | CP | 36 | TYR | 4.1 |
| 18 | BR | 21 | ILE | 4.1 |
| 20 | BT | 40 | GLU | 4.1 |
| 22 | CA | 1533 | C | 4.1 |
| 33 | CM | 105 | ILE | 4.1 |
| 21 | AU | 55 | ARG | 4.1 |
| 27 | CF | 30 | ARG | 4.1 |
| 3 | BC | 96 | GLY | 4.1 |
| 25 | CD | 156 | PHE | 4.1 |
| 1 | AA | 89 | U | 4.1 |
| 1 | BA | 1341 | U | 4.1 |
| 13 | BM | 21 | SER | 4.1 |
| 14 | BN | 94 | PRO | 4.1 |
| 22 | CA | 1088 | A | 4.1 |
| 22 | CA | 2132 | U | 4.1 |
| 11 | BK | 76 | GLU | 4.1 |
| 26 | CE | 144 | GLU | 4.1 |
| 29 | DH | 45 | GLU | 4.1 |
| 40 | CT | 51 | LEU | 4.1 |
| 1 | BA | 1134 | G | 4.1 |
| 1 | BA | 1209 | C | 4.1 |
| 22 | CA | 1045 | C | 4.1 |
| 17 | BQ | 65 | ARG | 4.1 |
| 29 | CH | 133 | GLN | 4.1 |
| 39 | CS | 101 | ILE | 4.1 |
| 22 | CA | 1060 | U | 4.1 |
| 31 | CK | 83 | GLY | 4.1 |
| 53 | DA | 884 | U | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 22 | CA | 345 | A | 4.1 |
| 43 | CW | 7 | GLU | 4.1 |
| 48 | C1 | 27 | SER | 4.1 |
| 2 | AB | 16 | PHE | 4.1 |
| 9 | AI | 20 | PHE | 4.1 |
| 21 | AU | 19 | PHE | 4.1 |
| 21 | BU | 12 | PHE | 4.1 |
| 24 | CC | 61 | ALA | 4.1 |
| 28 | CG | 54 | PRO | 4.1 |
| 29 | CH | 64 | ALA | 4.1 |
| 36 | CP | 11 | ALA | 4.1 |
| 2 | AB | 143 | LYS | 4.1 |
| 2 | BB | 148 | LEU | 4.1 |
| 2 | BB | 211 | THR | 4.1 |
| 19 | AS | 64 | ASP | 4.1 |
| 28 | CG | 88 | GLN | 4.1 |
| 28 | CG | 158 | LYS | 4.1 |
| 3 | BC | 153 | VAL | 4.1 |
| 17 | BQ | 73 | TRP | 4.1 |
| 52 | C5 | 25 | VAL | 4.1 |
| 3 | AC | 101 | ILE | 4.1 |
| 20 | BT | 67 | ILE | 4.1 |
| 22 | CA | 320 | A | 4.1 |
| 1 | BA | 214 | C | 4.1 |
| 23 | CB | 38 | C | 4.1 |
| 13 | BM | 114 | LYS | 4.1 |
| 14 | BN | 7 | LYS | 4.1 |
| 14 | BN | 99 | ALA | 4.1 |
| 22 | CA | 653 | U | 4.1 |
| 37 | CQ | 111 | LYS | 4.1 |
| 7 | BG | 126 | ASP | 4.1 |
| 40 | CT | 109 | ASP | 4.1 |
| 28 | CG | 36 | THR | 4.1 |
| 48 | C1 | 26 | THR | 4.1 |
| 53 | DA | 2128 | G | 4.1 |
| 29 | DH | 90 | LEU | 4.1 |
| 55 | DI | 5 | LEU | 4.1 |
| 13 | AM | 6 | GLY | 4.1 |
| 22 | CA | 101 | A | 4.1 |
| 22 | CA | 278 | A | 4.1 |
| 33 | CM | 21 | ARG | 4.1 |
| 19 | AS | 17 | LYS | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 22 | CA | 897 | C | 4.1 |
| 22 | CA | 2795 | C | 4.1 |
| 24 | CC | 78 | VAL | 4.1 |
| 28 | CG | 90 | VAL | 4.1 |
| 33 | CM | 127 | VAL | 4.1 |
| 53 | DA | 846 | U | 4.1 |
| 5 | BE | 30 | ILE | 4.1 |
| 7 | BG | 16 | PRO | 4.1 |
| 39 | CS | 74 | ILE | 4.1 |
| 54 | DD | 152 | PRO | 4.1 |
| 40 | CT | 62 | ASP | 4.1 |
| 3 | BC | 46 | GLU | 4.1 |
| 25 | CD | 206 | ALA | 4.1 |
| 29 | DH | 129 | GLU | 4.1 |
| 1 | BA | 1007 | U | 4.1 |
| 9 | AI | 61 | LEU | 4.1 |
| 29 | CH | 116 | ARG | 4.0 |
| 37 | CQ | 40 | LEU | 4.1 |
| 39 | CS | 60 | LYS | 4.0 |
| 41 | CU | 44 | LYS | 4.0 |
| 31 | CK | 138 | GLN | 4.0 |
| 45 | CY | 35 | SER | 4.0 |
| 46 | CZ | 34 | SER | 4.0 |
| 17 | AQ | 52 | GLU | 4.0 |
| 11 | BK | 77 | TYR | 4.0 |
| 21 | AU | 14 | VAL | 4.0 |
| 21 | BU | 53 | VAL | 4.0 |
| 9 | AI | 30 | ILE | 4.0 |
| 38 | CR | 2 | ALA | 4.0 |
| 1 | BA | 1002 | G | 4.0 |
| 1 | BA | 1139 | G | 4.0 |
| 22 | CA | 2304 | G | 4.0 |
| 8 | BH | 66 | PHE | 4.0 |
| 9 | AI | 26 | GLY | 4.0 |
| 13 | AM | 26 | GLY | 4.0 |
| 16 | BP | 39 | PHE | 4.0 |
| 25 | CD | 163 | GLY | 4.0 |
| 33 | CM | 66 | PHE | 4.0 |
| 39 | CS | 67 | GLY | 4.0 |
| 23 | CB | 49 | C | 4.0 |
| 53 | DA | 2173 | A | 4.0 |
| 30 | CJ | 108 | GLU | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 36 | CP | 55 | GLU | 4.0 |
| 33 | CM | 57 | LEU | 4.0 |
| 40 | CT | 46 | LEU | 4.0 |
| 8 | AH | 48 | ASP | 4.0 |
| 9 | AI | 128 | SER | 4.0 |
| 25 | CD | 181 | ASP | 4.0 |
| 55 | DI | 15 | VAL | 4.0 |
| 2 | AB | 137 | ARG | 4.0 |
| 3 | BC | 126 | ARG | 4.0 |
| 15 | AO | 11 | ILE | 4.0 |
| 20 | BT | 83 | ILE | 4.0 |
| 33 | CM | 75 | ALA | 4.0 |
| 1 | BA | 1004 | A | 4.0 |
| 1 | BA | 1236 | A | 4.0 |
| 1 | BA | 1331 | G | 4.0 |
| 22 | CA | 619 | G | 4.0 |
| 22 | CA | 1496 | A | 4.0 |
| 23 | CB | 51 | G | 4.0 |
| 24 | CC | 57 | GLY | 4.0 |
| 2 | BB | 205 | ASP | 4.0 |
| 3 | BC | 83 | ASP | 4.0 |
| 36 | CP | 93 | ASP | 4.0 |
| 1 | BA | 473 | U | 4.0 |
| 1 | BA | 957 | U | 4.0 |
| 53 | DA | 1066 | U | 4.0 |
| 13 | AM | 83 | LEU | 4.0 |
| 15 | BO | 87 | LEU | 4.0 |
| 46 | CZ | 28 | LEU | 4.0 |
| 46 | CZ | 43 | LEU | 4.0 |
| 15 | BO | 10 | LYS | 4.0 |
| 55 | DI | 62 | ARG | 4.0 |
| 14 | BN | 84 | VAL | 4.0 |
| 32 | CL | 61 | VAL | 4.0 |
| 53 | DA | 2145 | C | 4.0 |
| 1 | AA | 1009 | U | 4.0 |
| 22 | CA | 2183 | A | 4.0 |
| 36 | CP | 44 | GLY | 4.0 |
| 53 | DA | 1088 | A | 4.0 |
| 1 | BA | 144 | G | 4.0 |
| 1 | BA | 1015 | G | 4.0 |
| 22 | CA | 1062 | G | 4.0 |
| 53 | DA | 2102 | G | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 11 | AK | 17 | SER | 4.0 |
| 17 | BQ | 4 | LYS | 4.0 |
| 42 | CV | 97 | LYS | 4.0 |
| 27 | DF | 77 | PHE | 4.0 |
| 35 | CO | 71 | ARG | 4.0 |
| 41 | CU | 92 | ASN | 4.0 |
| 44 | CX | 26 | PHE | 4.0 |
| 3 | BC | 175 | LEU | 4.0 |
| 54 | DD | 138 | LEU | 4.0 |
| 1 | AA | 88 | U | 4.0 |
| 1 | BA | 250 | A | 4.0 |
| 2 | AB | 8 | ASP | 4.0 |
| 9 | BI | 17 | ALA | 4.0 |
| 22 | CA | 1077 | A | 4.0 |
| 9 | AI | 27 | LYS | 4.0 |
| 19 | BS | 77 | THR | 4.0 |
| 2 | BB | 56 | GLU | 4.0 |
| 29 | CH | 137 | GLU | 4.0 |
| 20 | BT | 52 | ASN | 4.0 |
| 1 | BA | 1212 | U | 4.0 |
| 29 | DH | 46 | PHE | 4.0 |
| 28 | CG | 39 | ASP | 4.0 |
| 38 | CR | 26 | GLY | 4.0 |
| 7 | AG | 134 | ALA | 4.0 |
| 35 | CO | 120 | GLU | 4.0 |
| 55 | DI | 63 | ALA | 4.0 |
| 1 | BA | 1255 | G | 4.0 |
| 1 | BA | 1358 | U | 4.0 |
| 27 | CF | 127 | ASN | 4.0 |
| 29 | CH | 40 | THR | 4.0 |
| 35 | CO | 36 | THR | 4.0 |
| 52 | C5 | 7 | VAL | 4.0 |
| 9 | AI | 21 | ILE | 4.0 |
| 14 | AN | 18 | ASP | 3.9 |
| 1 | AA | 1441 | A | 3.9 |
| 22 | CA | 1046 | A | 3.9 |
| 22 | CA | 1590 | A | 3.9 |
| 29 | DH | 87 | GLU | 3.9 |
| 2 | BB | 17 | GLY | 3.9 |
| 19 | AS | 74 | PHE | 3.9 |
| 28 | CG | 71 | LEU | 3.9 |
| 23 | CB | 9 | G | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | AB | 128 | LYS | 3.9 |
| 26 | CE | 32 | VAL | 3.9 |
| 38 | CR | 34 | VAL | 3.9 |
| 50 | D3 | 46 | LYS | 3.9 |
| 55 | DI | 85 | VAL | 3.9 |
| 14 | BN | 26 | GLU | 3.9 |
| 31 | DK | 84 | ILE | 3.9 |
| 22 | CA | 2114 | A | 3.9 |
| 22 | CA | 2131 | U | 3.9 |
| 22 | CA | 2135 | A | 3.9 |
| 28 | CG | 66 | GLY | 3.9 |
| 6 | BF | 1 | MET | 3.9 |
| 13 | AM | 63 | PHE | 3.9 |
| 46 | CZ | 45 | GLN | 3.9 |
| 3 | BC | 180 | ALA | 3.9 |
| 20 | BT | 17 | ALA | 3.9 |
| 27 | CF | 70 | ALA | 3.9 |
| 42 | CV | 44 | LYS | 3.9 |
| 16 | BP | 50 | THR | 3.9 |
| 22 | CA | 1730 | C | 3.9 |
| 22 | CA | 1733 | G | 3.9 |
| 39 | CS | 94 | THR | 3.9 |
| 53 | DA | 357 | C | 3.9 |
| 6 | BF | 18 | VAL | 3.9 |
| 49 | C2 | 42 | VAL | 3.9 |
| 9 | BI | 18 | ARG | 3.9 |
| 13 | BM | 87 | ARG | 3.9 |
| 53 | DA | 2183 | A | 3.9 |
| 28 | CG | 19 | ILE | 3.9 |
| 34 | CN | 73 | ILE | 3.9 |
| 9 | BI | 25 | ASN | 3.9 |
| 12 | AL | 123 | LYS | 3.9 |
| 29 | CH | 8 | LYS | 3.9 |
| 37 | DQ | 66 | ASN | 3.9 |
| 6 | BF | 65 | GLU | 3.9 |
| 1 | AA | 1037 | C | 3.9 |
| 9 | BI | 93 | SER | 3.9 |
| 13 | AM | 56 | LEU | 3.9 |
| 22 | CA | 314 | C | 3.9 |
| 22 | CA | 351 | C | 3.9 |
| 22 | CA | 898 | C | 3.9 |
| 22 | CA | 1105 | U | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 32 | CL | 109 | SER | 3.9 |
| 53 | DA | 140 | C | 3.9 |
| 53 | DA | 1173 | U | 3.9 |
| 4 | AD | 20 | PHE | 3.9 |
| 9 | AI | 94 | LEU | 3.9 |
| 10 | AJ | 91 | ASP | 3.9 |
| 20 | BT | 47 | ALA | 3.9 |
| 28 | CG | 137 | ASP | 3.9 |
| 29 | CH | 69 | ALA | 3.9 |
| 37 | DQ | 114 | LEU | 3.9 |
| 1 | BA | 161 | A | 3.9 |
| 22 | CA | 63 | A | 3.9 |
| 22 | CA | 1551 | A | 3.9 |
| 14 | BN | 101 | TRP | 3.9 |
| 10 | AJ | 84 | VAL | 3.9 |
| 26 | CE | 97 | ASN | 3.9 |
| 39 | CS | 44 | GLY | 3.9 |
| 3 | BC | 105 | GLU | 3.9 |
| 29 | CH | 70 | GLU | 3.9 |
| 36 | CP | 46 | GLU | 3.9 |
| 43 | CW | 63 | ILE | 3.9 |
| 7 | AG | 144 | MET | 3.9 |
| 2 | BB | 43 | LEU | 3.9 |
| 1 | BA | 975 | A | 3.9 |
| 2 | AB | 152 | LYS | 3.9 |
| 22 | CA | 2801 | G | 3.9 |
| 30 | CJ | 72 | LYS | 3.9 |
| 37 | CQ | 6 | LYS | 3.9 |
| 37 | CQ | 20 | PHE | 3.9 |
| 53 | DA | 1062 | G | 3.9 |
| 53 | DA | 2186 | G | 3.9 |
| 22 | CA | 1097 | U | 3.9 |
| 22 | CA | 2796 | U | 3.9 |
| 24 | CC | 251 | GLN | 3.9 |
| 26 | CE | 198 | GLU | 3.9 |
| 42 | CV | 99 | ASN | 3.9 |
| 44 | CX | 65 | GLY | 3.9 |
| 49 | C2 | 46 | HIS | 3.9 |
| 9 | AI | 72 | ILE | 3.9 |
| 25 | CD | 27 | ILE | 3.9 |
| 34 | CN | 126 | ILE | 3.9 |
| 36 | CP | 52 | SER | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | BB | 174 | LYS | 3.9 |
| 3 | AC | 38 | LYS | 3.9 |
| 1 | BA | 1321 | U | 3.9 |
| 22 | CA | 2118 | U | 3.9 |
| 2 | BB | 76 | ALA | 3.9 |
| 41 | CU | 61 | LEU | 3.9 |
| 48 | D1 | 9 | THR | 3.9 |
| 2 | AB | 162 | PHE | 3.9 |
| 25 | CD | 198 | GLY | 3.9 |
| 9 | AI | 91 | ASP | 3.9 |
| 45 | CY | 50 | ARG | 3.9 |
| 24 | CC | 228 | VAL | 3.9 |
| 54 | DD | 155 | VAL | 3.9 |
| 2 | AB | 40 | ILE | 3.8 |
| 36 | CP | 87 | ILE | 3.8 |
| 32 | CL | 48 | PRO | 3.8 |
| 1 | BA | 1003 | G | 3.8 |
| 22 | CA | 2735 | G | 3.8 |
| 1 | BA | 1397 | C | 3.8 |
| 22 | CA | 1582 | C | 3.8 |
| 29 | DH | 13 | GLY | 3.8 |
| 2 | AB | 63 | ARG | 3.8 |
| 2 | BB | 45 | LYS | 3.8 |
| 7 | BG | 138 | ARG | 3.8 |
| 41 | CU | 9 | LYS | 3.8 |
| 2 | BB | 5 | SER | 3.8 |
| 31 | CK | 136 | GLN | 3.8 |
| 34 | CN | 105 | MET | 3.8 |
| 2 | BB | 47 | VAL | 3.8 |
| 37 | CQ | 80 | VAL | 3.8 |
| 9 | BI | 51 | PRO | 3.8 |
| 25 | CD | 32 | ASN | 3.8 |
| 1 | AA | 1029 | U | 3.8 |
| 11 | AK | 66 | ALA | 3.8 |
| 11 | AK | 97 | ILE | 3.8 |
| 20 | BT | 12 | ILE | 3.8 |
| 35 | CO | 112 | TYR | 3.8 |
| 2 | AB | 138 | THR | 3.8 |
| 45 | CY | 77 | LYS | 3.8 |
| 54 | DD | 121 | THR | 3.8 |
| 1 | AA | 204 | G | 3.8 |
| 27 | CF | 166 | GLY | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 28 | CG | 61 | GLY | 3.8 |
| 17 | BQ | 8 | LEU | 3.8 |
| 19 | AS | 15 | LEU | 3.8 |
| 29 | CH | 91 | PHE | 3.8 |
| 31 | CK | 119 | PHE | 3.8 |
| 51 | C4 | 61 | CYS | 3.8 |
| 1 | BA | 1332 | A | 3.8 |
| 25 | CD | 1 | MET | 3.8 |
| 53 | DA | 1070 | A | 3.8 |
| 55 | DI | 103 | ASN | 3.8 |
| 17 | AQ | 4 | LYS | 3.8 |
| 51 | C4 | 19 | LYS | 3.8 |
| 7 | BG | 2 | PRO | 3.8 |
| 7 | BG | 90 | GLU | 3.8 |
| 24 | CC | 144 | VAL | 3.8 |
| 25 | CD | 183 | GLU | 3.8 |
| 27 | CF | 98 | GLU | 3.8 |
| 32 | CL | 122 | VAL | 3.8 |
| 48 | D1 | 3 | VAL | 3.8 |
| 9 | BI | 70 | GLY | 3.8 |
| 10 | AJ | 23 | ALA | 3.8 |
| 16 | BP | 65 | ALA | 3.8 |
| 25 | CD | 197 | THR | 3.8 |
| 31 | CK | 93 | ILE | 3.8 |
| 40 | CT | 4 | ILE | 3.8 |
| 43 | CW | 29 | ILE | 3.8 |
| 44 | CX | 43 | THR | 3.8 |
| 3 | BC | 178 | LEU | 3.8 |
| 24 | DC | 205 | LEU | 3.8 |
| 4 | BD | 45 | LYS | 3.8 |
| 50 | C3 | 26 | ASN | 3.8 |
| 1 | BA | 83 | C | 3.8 |
| 22 | CA | 1727 | C | 3.8 |
| 7 | BG | 55 | GLY | 3.8 |
| 1 | BA | 202 | G | 3.8 |
| 22 | CA | 1587 | G | 3.8 |
| 3 | AC | 89 | LYS | 3.8 |
| 10 | AJ | 100 | ILE | 3.8 |
| 17 | BQ | 34 | TYR | 3.8 |
| 18 | BR | 30 | LYS | 3.8 |
| 38 | DR | 40 | ILE | 3.8 |
| 40 | CT | 48 | LYS | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 55 | DI | 51 | TYR | 3.8 |
| 1 | BA | 78 | A | 3.8 |
| 22 | CA | 1383 | A | 3.8 |
| 7 | BG | 119 | ARG | 3.8 |
| 13 | AM | 57 | ARG | 3.8 |
| 29 | CH | 117 | LEU | 3.8 |
| 2 | AB | 154 | MET | 3.8 |
| 9 | AI | 57 | MET | 3.8 |
| 22 | CA | 2130 | U | 3.8 |
| 2 | AB | 150 | GLY | 3.8 |
| 28 | CG | 53 | GLY | 3.8 |
| 14 | BN | 64 | CYS | 3.8 |
| 48 | C1 | 37 | LYS | 3.8 |
| 11 | BK | 103 | ALA | 3.8 |
| 21 | BU | 52 | ALA | 3.8 |
| 24 | CC | 65 | VAL | 3.8 |
| 31 | CK | 117 | ALA | 3.8 |
| 34 | CN | 116 | ALA | 3.8 |
| 38 | CR | 115 | ALA | 3.8 |
| 22 | CA | 2133 | G | 3.8 |
| 53 | DA | 359 | G | 3.8 |
| 21 | BU | 55 | ARG | 3.8 |
| 22 | CA | 1420 | A | 3.8 |
| 24 | CC | 239 | ASN | 3.8 |
| 36 | CP | 102 | ARG | 3.8 |
| 7 | BG | 42 | ILE | 3.8 |
| 11 | BK | 23 | ILE | 3.8 |
| 31 | CK | 53 | TYR | 3.8 |
| 43 | CW | 70 | ILE | 3.8 |
| 3 | BC | 12 | LEU | 3.8 |
| 9 | BI | 46 | MET | 3.8 |
| 10 | BJ | 71 | LEU | 3.8 |
| 28 | CG | 44 | LYS | 3.8 |
| 4 | AD | 163 | GLU | 3.8 |
| 16 | BP | 10 | GLY | 3.8 |
| 2 | AB | 208 | ARG | 3.7 |
| 1 | AA | 1024 | G | 3.7 |
| 1 | BA | 1034 | G | 3.7 |
| 1 | BA | 1324 | A | 3.7 |
| 6 | BF | 32 | ALA | 3.7 |
| 9 | AI | 101 | ALA | 3.7 |
| 15 | AO | 18 | ASP | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 17 | BQ | 46 | VAL | 3.7 |
| 22 | CA | 74 | A | 3.7 |
| 22 | CA | 1444 | G | 3.7 |
| 35 | DO | 125 | ALA | 3.7 |
| 24 | CC | 94 | VAL | 3.7 |
| 39 | CS | 47 | VAL | 3.7 |
| 53 | DA | 358 | U | 3.7 |
| 29 | CH | 7 | ASP | 3.7 |
| 38 | CR | 47 | TYR | 3.7 |
| 40 | CT | 103 | ILE | 3.7 |
| 7 | AG | 58 | GLU | 3.7 |
| 3 | BC | 60 | PRO | 3.7 |
| 4 | AD | 176 | GLY | 3.7 |
| 5 | BE | 15 | LEU | 3.7 |
| 6 | BF | 67 | PRO | 3.7 |
| 13 | AM | 51 | GLY | 3.7 |
| 18 | AR | 68 | LEU | 3.7 |
| 33 | CM | 53 | GLY | 3.7 |
| 2 | AB | 30 | PHE | 3.7 |
| 22 | CA | 1048 | A | 3.7 |
| 27 | CF | 168 | ALA | 3.7 |
| 28 | CG | 67 | THR | 3.7 |
| 35 | CO | 72 | ASP | 3.7 |
| 1 | AA | 211 | G | 3.7 |
| 14 | AN | 44 | ALA | 3.7 |
| 16 | BP | 82 | ALA | 3.7 |
| 13 | BM | 27 | LYS | 3.7 |
| 22 | CA | 489 | G | 3.7 |
| 22 | CA | 1543 | G | 3.7 |
| 50 | C3 | 23 | ALA | 3.7 |
| 25 | CD | 38 | LYS | 3.7 |
| 42 | CV | 92 | LYS | 3.7 |
| 4 | AD | 142 | VAL | 3.7 |
| 24 | DC | 17 | VAL | 3.7 |
| 1 | BA | 1364 | U | 3.7 |
| 22 | CA | 2423 | U | 3.7 |
| 40 | CT | 38 | TYR | 3.7 |
| 48 | C1 | 51 | GLY | 3.7 |
| 13 | BM | 110 | LYS | 3.7 |
| 15 | AO | 2 | SER | 3.7 |
| 25 | CD | 99 | GLU | 3.7 |
| 9 | BI | 9 | THR | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 16 | BP | 73 | ALA | 3.7 |
| 18 | AR | 27 | ALA | 3.7 |
| 29 | CH | 46 | PHE | 3.7 |
| 22 | CA | 367 | G | 3.7 |
| 22 | CA | 2353 | G | 3.7 |
| 22 | CA | 290 | U | 3.7 |
| 22 | CA | 1412 | U | 3.7 |
| 27 | CF | 5 | HIS | 3.7 |
| 33 | CM | 35 | HIS | 3.7 |
| 3 | AC | 90 | VAL | 3.7 |
| 45 | CY | 47 | VAL | 3.7 |
| 51 | D4 | 50 | VAL | 3.7 |
| 25 | CD | 105 | LYS | 3.7 |
| 14 | BN | 93 | ILE | 3.7 |
| 53 | DA | 142 | A | 3.7 |
| 3 | BC | 87 | LEU | 3.7 |
| 11 | AK | 82 | LEU | 3.7 |
| 39 | CS | 29 | THR | 3.7 |
| 1 | AA | 1033 | G | 3.7 |
| 1 | BA | 203 | G | 3.7 |
| 28 | CG | 145 | ALA | 3.7 |
| 29 | CH | 84 | ALA | 3.7 |
| 11 | BK | 61 | PHE | 3.7 |
| 34 | CN | 28 | PHE | 3.7 |
| 46 | CZ | 26 | PHE | 3.7 |
| 3 | BC | 74 | GLY | 3.7 |
| 13 | BM | 50 | GLU | 3.7 |
| 29 | DH | 57 | LYS | 3.7 |
| 1 | AA | 207 | C | 3.7 |
| 1 | BA | 1263 | C | 3.7 |
| 6 | BF | 10 | VAL | 3.7 |
| 19 | AS | 43 | ASN | 3.7 |
| 24 | DC | 213 | TRP | 3.7 |
| 29 | CH | 134 | VAL | 3.7 |
| 38 | CR | 61 | TRP | 3.7 |
| 44 | CX | 67 | VAL | 3.7 |
| 54 | DD | 122 | VAL | 3.7 |
| 53 | DA | 1061 | U | 3.7 |
| 1 | BA | 1005 | A | 3.7 |
| 2 | BB | 200 | ILE | 3.7 |
| 3 | BC | 20 | SER | 3.7 |
| 2 | BB | 68 | LEU | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 11 | AK | 100 | LEU | 3.7 |
| 17 | BQ | 11 | ARG | 3.7 |
| 25 | CD | 179 | ARG | 3.7 |
| 36 | CP | 48 | LEU | 3.7 |
| 7 | BG | 142 | HIS | 3.7 |
| 29 | DH | 79 | THR | 3.7 |
| 1 | AA | 1018 | G | 3.7 |
| 1 | BA | 1268 | G | 3.7 |
| 24 | DC | 211 | ALA | 3.7 |
| 27 | CF | 160 | ALA | 3.7 |
| 31 | CK | 20 | ALA | 3.7 |
| 22 | CA | 358 | U | 3.7 |
| 1 | BA | 1317 | C | 3.7 |
| 22 | CA | 163 | C | 3.7 |
| 22 | CA | 2300 | C | 3.7 |
| 27 | CF | 131 | GLY | 3.7 |
| 54 | DD | 144 | GLY | 3.7 |
| 1 | BA | 1167 | A | 3.7 |
| 53 | DA | 2184 | A | 3.7 |
| 4 | AD | 101 | VAL | 3.7 |
| 2 | AB | 147 | SER | 3.7 |
| 2 | BB | 222 | ARG | 3.7 |
| 38 | CR | 33 | ARG | 3.7 |
| 11 | BK | 80 | LYS | 3.7 |
| 29 | DH | 4 | ILE | 3.7 |
| 33 | DM | 35 | HIS | 3.7 |
| 53 | DA | 2182 | U | 3.7 |
| 29 | CH | 58 | LEU | 3.7 |
| 30 | DJ | 118 | THR | 3.7 |
| 33 | CM | 27 | LEU | 3.7 |
| 34 | CN | 20 | LEU | 3.7 |
| 35 | CO | 98 | LEU | 3.7 |
| 38 | CR | 18 | LEU | 3.7 |
| 1 | BA | 260 | G | 3.7 |
| 11 | AK | 21 | ALA | 3.7 |
| 22 | CA | 2143 | C | 3.6 |
| 25 | CD | 119 | ALA | 3.7 |
| 51 | C4 | 65 | ALA | 3.7 |
| 2 | AB | 17 | GLY | 3.6 |
| 44 | CX | 34 | GLY | 3.6 |
| 53 | DA | 547 | A | 3.6 |
| 48 | C1 | 15 | MET | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 7 | AG | 70 | ARG | 3.6 |
| 19 | AS | 28 | LYS | 3.6 |
| 20 | AT | 5 | LYS | 3.6 |
| 37 | CQ | 72 | ARG | 3.6 |
| 1 | BA | 479 | U | 3.6 |
| 8 | BH | 2 | SER | 3.6 |
| 22 | CA | 1742 | U | 3.6 |
| 53 | DA | 2131 | U | 3.6 |
| 19 | AS | 45 | ILE | 3.6 |
| 22 | CA | 366 | C | 3.6 |
| 33 | CM | 128 | THR | 3.6 |
| 1 | AA | 462 | G | 3.6 |
| 1 | BA | 1041 | G | 3.6 |
| 6 | AF | 61 | LEU | 3.6 |
| 24 | CC | 105 | LEU | 3.6 |
| 38 | CR | 38 | ALA | 3.6 |
| 54 | DD | 119 | ALA | 3.6 |
| 9 | BI | 89 | GLU | 3.6 |
| 22 | CA | 89 | A | 3.6 |
| 22 | CA | 1486 | U | 3.6 |
| 24 | CC | 6 | CYS | 3.6 |
| 26 | CE | 125 | SER | 3.6 |
| 39 | CS | 91 | GLN | 3.6 |
| 3 | BC | 116 | VAL | 3.6 |
| 22 | CA | 336 | C | 3.6 |
| 22 | CA | 360 | U | 3.6 |
| 17 | AQ | 54 | GLY | 3.6 |
| 24 | CC | 246 | THR | 3.6 |
| 27 | CF | 69 | LYS | 3.6 |
| 31 | CK | 68 | LYS | 3.6 |
| 47 | C0 | 39 | GLU | 3.6 |
| 48 | C1 | 53 | LYS | 3.6 |
| 53 | DA | 545 | U | 3.6 |
| 53 | DA | 1078 | U | 3.6 |
| 2 | AB | 171 | ILE | 3.6 |
| 2 | BB | 10 | LEU | 3.6 |
| 3 | AC | 77 | ILE | 3.6 |
| 8 | BH | 59 | LEU | 3.6 |
| 10 | AJ | 76 | ILE | 3.6 |
| 14 | AN | 53 | ARG | 3.6 |
| 22 | CA | 1860 | G | 3.6 |
| 25 | CD | 188 | LEU | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 28 | CG | 141 | ILE | 3.6 |
| 31 | CK | 95 | ARG | 3.6 |
| 21 | AU | 16 | LEU | 3.6 |
| 33 | CM | 8 | PRO | 3.6 |
| 33 | CM | 103 | ILE | 3.6 |
| 33 | CM | 125 | LEU | 3.6 |
| 37 | CQ | 114 | LEU | 3.6 |
| 25 | CD | 97 | SER | 3.6 |
| 13 | BM | 42 | ASP | 3.6 |
| 10 | BJ | 49 | PHE | 3.6 |
| 53 | DA | 897 | C | 3.6 |
| 19 | AS | 20 | GLU | 3.6 |
| 29 | DH | 141 | LYS | 3.6 |
| 40 | CT | 61 | ASN | 3.6 |
| 44 | CX | 62 | LYS | 3.6 |
| 6 | BF | 60 | VAL | 3.6 |
| 15 | BO | 75 | VAL | 3.6 |
| 24 | CC | 184 | VAL | 3.6 |
| 29 | DH | 51 | ARG | 3.6 |
| 31 | CK | 62 | VAL | 3.6 |
| 38 | CR | 13 | ARG | 3.6 |
| 1 | AA | 1005 | A | 3.6 |
| 2 | BB | 46 | THR | 3.6 |
| 13 | AM | 38 | GLY | 3.6 |
| 22 | CA | 1735 | A | 3.6 |
| 33 | DM | 30 | THR | 3.6 |
| 55 | DI | 32 | GLY | 3.6 |
| 3 | BC | 71 | ALA | 3.6 |
| 28 | CG | 119 | ALA | 3.6 |
| 30 | DJ | 77 | ALA | 3.6 |
| 55 | DI | 102 | ALA | 3.6 |
| 10 | AJ | 25 | ILE | 3.6 |
| 14 | BN | 96 | LEU | 3.6 |
| 36 | CP | 98 | GLN | 3.6 |
| 51 | C4 | 4 | ILE | 3.6 |
| 22 | CA | 1061 | U | 3.6 |
| 42 | CV | 100 | SER | 3.6 |
| 1 | BA | 87 | C | 3.6 |
| 1 | BA | 1137 | C | 3.6 |
| 3 | AC | 170 | GLU | 3.6 |
| 7 | AG | 63 | GLU | 3.6 |
| 29 | CH | 127 | GLU | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | DH | 112 | LYS | 3.6 |
| 34 | CN | 84 | LYS | 3.6 |
| 21 | AU | 34 | ARG | 3.6 |
| 26 | CE | 114 | ARG | 3.6 |
| 2 | BB | 180 | GLY | 3.6 |
| 3 | BC | 197 | GLY | 3.6 |
| 9 | AI | 117 | GLY | 3.6 |
| 22 | CA | 354 | A | 3.6 |
| 22 | CA | 404 | A | 3.6 |
| 10 | BJ | 84 | VAL | 3.6 |
| 47 | C0 | 41 | THR | 3.6 |
| 7 | AG | 129 | GLU | 3.6 |
| 12 | BL | 2 | ALA | 3.6 |
| 17 | BQ | 24 | ALA | 3.6 |
| 55 | DI | 19 | ALA | 3.6 |
| 10 | AJ | 101 | SER | 3.6 |
| 2 | BB | 129 | LEU | 3.6 |
| 26 | DE | 73 | ILE | 3.6 |
| 27 | CF | 36 | LEU | 3.6 |
| 55 | DI | 4 | ASN | 3.6 |
| 45 | CY | 57 | ARG | 3.6 |
| 22 | CA | 1224 | U | 3.6 |
| 32 | CL | 101 | GLY | 3.6 |
| 54 | DD | 147 | GLY | 3.6 |
| 3 | BC | 26 | THR | 3.6 |
| 20 | BT | 76 | LYS | 3.6 |
| 25 | CD | 112 | THR | 3.6 |
| 1 | BA | 457 | G | 3.6 |
| 1 | BA | 474 | G | 3.6 |
| 22 | CA | 1052 | C | 3.6 |
| 22 | CA | 2808 | G | 3.6 |
| 37 | CQ | 46 | VAL | 3.6 |
| 7 | BG | 147 | ALA | 3.6 |
| 9 | AI | 121 | ALA | 3.6 |
| 15 | BO | 4 | SER | 3.6 |
| 24 | CC | 122 | ALA | 3.6 |
| 38 | CR | 63 | ALA | 3.6 |
| 39 | CS | 61 | ALA | 3.6 |
| 53 | DA | 1728 | C | 3.6 |
| 2 | BB | 51 | ASN | 3.6 |
| 10 | BJ | 72 | ARG | 3.6 |
| 27 | CF | 24 | SER | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 28 | CG | 149 | ARG | 3.6 |
| 29 | CH | 73 | ASN | 3.6 |
| 1 | AA | 1010 | U | 3.5 |
| 1 | BA | 956 | U | 3.5 |
| 4 | BD | 55 | LEU | 3.5 |
| 23 | CB | 40 | U | 3.5 |
| 28 | CG | 72 | LEU | 3.5 |
| 13 | AM | 47 | GLU | 3.5 |
| 17 | BQ | 52 | GLU | 3.5 |
| 22 | CA | 1069 | A | 3.5 |
| 23 | CB | 108 | A | 3.5 |
| 29 | CH | 60 | GLU | 3.5 |
| 3 | BC | 194 | GLY | 3.5 |
| 28 | CG | 114 | ASP | 3.5 |
| 2 | AB | 198 | PHE | 3.5 |
| 29 | CH | 29 | PHE | 3.5 |
| 53 | DA | 2177 | C | 3.5 |
| 9 | BI | 41 | ARG | 3.5 |
| 32 | CL | 98 | ARG | 3.5 |
| 54 | DD | 118 | PHE | 3.5 |
| 22 | CA | 307 | G | 3.5 |
| 22 | CA | 1182 | G | 3.5 |
| 22 | CA | 1718 | G | 3.5 |
| 22 | CA | 2136 | G | 3.5 |
| 2 | AB | 39 | HIS | 3.5 |
| 16 | AP | 58 | ALA | 3.5 |
| 33 | CM | 113 | ALA | 3.5 |
| 35 | CO | 60 | VAL | 3.5 |
| 38 | CR | 100 | VAL | 3.5 |
| 21 | AU | 54 | LYS | 3.5 |
| 1 | BA | 478 | A | 3.5 |
| 1 | BA | 1375 | A | 3.5 |
| 22 | CA | 1745 | A | 3.5 |
| 20 | AT | 65 | GLY | 3.5 |
| 25 | CD | 166 | GLY | 3.5 |
| 29 | DH | 15 | LEU | 3.5 |
| 32 | CL | 107 | LEU | 3.5 |
| 40 | CT | 23 | LEU | 3.5 |
| 1 | BA | 271 | C | 3.5 |
| 29 | CH | 123 | ARG | 3.5 |
| 6 | BF | 30 | THR | 3.5 |
| 7 | AG | 68 | ASN | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 41 | CU | 59 | ASN | 3.5 |
| 2 | BB | 191 | SER | 3.5 |
| 13 | AM | 50 | GLU | 3.5 |
| 47 | C0 | 52 | SER | 3.5 |
| 19 | BS | 10 | PHE | 3.5 |
| 33 | CM | 141 | LYS | 3.5 |
| 53 | DA | 1869 | G | 3.5 |
| 28 | CG | 123 | ALA | 3.5 |
| 32 | CL | 113 | MET | 3.5 |
| 2 | AB | 80 | VAL | 3.5 |
| 8 | BH | 110 | VAL | 3.5 |
| 24 | DC | 144 | VAL | 3.5 |
| 31 | CK | 124 | VAL | 3.5 |
| 52 | C5 | 3 | VAL | 3.5 |
| 3 | AC | 136 | ARG | 3.5 |
| 3 | BC | 58 | GLU | 3.5 |
| 38 | CR | 85 | LYS | 3.5 |
| 38 | DR | 32 | TYR | 3.5 |
| 11 | AK | 111 | THR | 3.5 |
| 21 | AU | 51 | SER | 3.5 |
| 1 | BA | 1442 | G | 3.5 |
| 22 | CA | 175 | G | 3.5 |
| 23 | CB | 33 | G | 3.5 |
| 1 | BA | 1010 | U | 3.5 |
| 26 | CE | 141 | MET | 3.5 |
| 29 | CH | 86 | ASP | 3.5 |
| 38 | DR | 35 | ALA | 3.5 |
| 54 | DD | 156 | PHE | 3.5 |
| 14 | BN | 68 | GLY | 3.5 |
| 33 | CM | 26 | GLY | 3.5 |
| 35 | CO | 96 | ARG | 3.5 |
| 51 | C4 | 36 | LYS | 3.5 |
| 28 | DG | 101 | ASN | 3.5 |
| 31 | CK | 109 | LEU | 3.5 |
| 7 | AG | 12 | ILE | 3.5 |
| 22 | CA | 153 | U | 3.5 |
| 29 | DH | 14 | SER | 3.5 |
| 31 | CK | 81 | ILE | 3.5 |
| 35 | CO | 34 | ILE | 3.5 |
| 38 | CR | 40 | ILE | 3.5 |
| 18 | AR | 51 | TYR | 3.5 |
| 1 | AA | 80 | A | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | CA | 230 | G | 3.5 |
| 22 | CA | 612 | G | 3.5 |
| 22 | CA | 1086 | A | 3.5 |
| 53 | DA | 2142 | A | 3.5 |
| 3 | AC | 92 | ALA | 3.5 |
| 13 | BM | 15 | ALA | 3.5 |
| 55 | DI | 13 | ALA | 3.5 |
| 1 | BA | 1208 | C | 3.5 |
| 35 | DO | 121 | LYS | 3.5 |
| 7 | BG | 68 | ASN | 3.5 |
| 26 | CE | 59 | PRO | 3.5 |
| 7 | BG | 140 | ASP | 3.5 |
| 19 | AS | 3 | ARG | 3.5 |
| 22 | CA | 1866 | A | 3.5 |
| 40 | CT | 74 | ILE | 3.5 |
| 41 | DU | 2 | ILE | 3.5 |
| 20 | BT | 19 | LYS | 3.5 |
| 30 | DJ | 82 | LYS | 3.5 |
| 44 | CX | 44 | LYS | 3.5 |
| 52 | C5 | 8 | LYS | 3.5 |
| 7 | AG | 85 | TYR | 3.5 |
| 22 | CA | 1408 | G | 3.5 |
| 49 | C2 | 49 | TYR | 3.5 |
| 11 | AK | 104 | GLY | 3.5 |
| 9 | AI | 25 | ASN | 3.5 |
| 24 | DC | 220 | VAL | 3.4 |
| 2 | AB | 205 | ASP | 3.4 |
| 8 | BH | 42 | GLU | 3.4 |
| 39 | CS | 102 | SER | 3.4 |
| 14 | BN | 12 | LYS | 3.4 |
| 27 | CF | 88 | LYS | 3.4 |
| 39 | CS | 92 | TRP | 3.4 |
| 45 | CY | 74 | ARG | 3.4 |
| 1 | BA | 845 | A | 3.4 |
| 22 | CA | 1808 | A | 3.4 |
| 22 | CA | 147 | C | 3.4 |
| 45 | CY | 22 | LEU | 3.4 |
| 47 | C0 | 8 | THR | 3.4 |
| 53 | DA | 1075 | C | 3.4 |
| 2 | AB | 149 | GLY | 3.4 |
| 24 | DC | 42 | GLY | 3.4 |
| 36 | CP | 104 | GLN | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 54 | DD | 117 | GLY | 3.4 |
| 7 | BG | 128 | ALA | 3.4 |
| 20 | BT | 37 | ALA | 3.4 |
| 41 | CU | 23 | ALA | 3.4 |
| 48 | C1 | 45 | ALA | 3.4 |
| 9 | BI | 112 | GLU | 3.4 |
| 19 | AS | 24 | GLU | 3.4 |
| 7 | BG | 35 | LYS | 3.4 |
| 13 | BM | 70 | ARG | 3.4 |
| 33 | CM | 14 | LYS | 3.4 |
| 1 | AA | 121 | U | 3.4 |
| 2 | AB | 86 | SER | 3.4 |
| 37 | CQ | 74 | PHE | 3.4 |
| 1 | AA | 77 | A | 3.4 |
| 7 | BG | 69 | VAL | 3.4 |
| 14 | AN | 34 | VAL | 3.4 |
| 38 | DR | 34 | VAL | 3.4 |
| 55 | DI | 33 | VAL | 3.4 |
| 1 | AA | 210 | C | 3.4 |
| 28 | CG | 139 | GLN | 3.4 |
| 43 | CW | 3 | THR | 3.4 |
| 2 | AB | 36 | ASN | 3.4 |
| 35 | CO | 83 | LEU | 3.4 |
| 1 | BA | 1215 | G | 3.4 |
| 2 | BB | 224 | GLY | 3.4 |
| 8 | AH | 44 | GLY | 3.4 |
| 9 | BI | 24 | GLY | 3.4 |
| 42 | CV | 69 | ASN | 3.4 |
| 1 | BA | 989 | U | 3.4 |
| 11 | BK | 45 | ALA | 3.4 |
| 31 | CK | 123 | LYS | 3.4 |
| 47 | C0 | 7 | ILE | 3.4 |
| 16 | BP | 31 | ARG | 3.4 |
| 17 | AQ | 53 | CYS | 3.4 |
| 25 | CD | 103 | ASP | 3.4 |
| 20 | BT | 75 | HIS | 3.4 |
| 12 | BL | 91 | PRO | 3.4 |
| 1 | AA | 468 | A | 3.4 |
| 1 | BA | 1257 | A | 3.4 |
| 22 | CA | 357 | C | 3.4 |
| 53 | DA | 885 | C | 3.4 |
| 53 | DA | 1076 | C | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 10 | AJ | 35 | GLN | 3.4 |
| 25 | CD | 68 | PHE | 3.4 |
| 2 | BB | 133 | GLU | 3.4 |
| 16 | BP | 21 | VAL | 3.4 |
| 16 | BP | 77 | GLU | 3.4 |
| 21 | AU | 24 | GLU | 3.4 |
| 29 | DH | 130 | VAL | 3.4 |
| 51 | C4 | 7 | VAL | 3.4 |
| 8 | BH | 120 | GLY | 3.4 |
| 22 | CA | 2111 | U | 3.4 |
| 36 | CP | 96 | GLY | 3.4 |
| 55 | DI | 109 | LYS | 3.4 |
| 1 | BA | 1300 | G | 3.4 |
| 21 | AU | 29 | LEU | 3.4 |
| 22 | CA | 543 | G | 3.4 |
| 22 | CA | 638 | G | 3.4 |
| 26 | CE | 27 | LEU | 3.4 |
| 33 | CM | 55 | MET | 3.4 |
| 38 | DR | 18 | LEU | 3.4 |
| 47 | C0 | 25 | LEU | 3.4 |
| 55 | DI | 81 | LEU | 3.4 |
| 15 | BO | 19 | ALA | 3.4 |
| 8 | BH | 36 | ILE | 3.4 |
| 21 | AU | 56 | HIS | 3.4 |
| 1 | AA | 1022 | A | 3.4 |
| 22 | CA | 256 | A | 3.4 |
| 52 | C5 | 28 | SER | 3.4 |
| 53 | DA | 892 | A | 3.4 |
| 30 | DJ | 130 | GLU | 3.4 |
| 1 | BA | 4 | U | 3.4 |
| 1 | BA | 1313 | U | 3.4 |
| 29 | DH | 43 | ASN | 3.4 |
| 31 | CK | 2 | LYS | 3.4 |
| 48 | C1 | 57 | LYS | 3.4 |
| 2 | BB | 183 | VAL | 3.4 |
| 14 | AN | 24 | ARG | 3.4 |
| 36 | CP | 30 | ARG | 3.4 |
| 37 | CQ | 105 | GLY | 3.4 |
| 38 | CR | 106 | PHE | 3.4 |
| 44 | CX | 64 | ASP | 3.4 |
| 5 | BE | 152 | MET | 3.4 |
| 43 | CW | 50 | MET | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | CA | 2308 | G | 3.4 |
| 25 | CD | 140 | HIS | 3.4 |
| 47 | D0 | 17 | LEU | 3.4 |
| 48 | C1 | 38 | HIS | 3.4 |
| 1 | BA | 841 | C | 3.4 |
| 23 | CB | 3 | C | 3.4 |
| 1 | BA | 1307 | U | 3.4 |
| 5 | AE | 61 | GLN | 3.4 |
| 11 | BK | 38 | GLN | 3.4 |
| 11 | BK | 102 | ALA | 3.4 |
| 28 | CG | 81 | GLU | 3.4 |
| 35 | CO | 114 | GLU | 3.4 |
| 22 | CA | 2340 | A | 3.4 |
| 23 | CB | 52 | A | 3.4 |
| 43 | CW | 10 | LYS | 3.4 |
| 49 | C2 | 13 | SER | 3.4 |
| 33 | DM | 23 | ILE | 3.4 |
| 35 | CO | 97 | ILE | 3.4 |
| 54 | DD | 125 | TRP | 3.4 |
| 6 | BF | 59 | TYR | 3.4 |
| 35 | CO | 22 | ARG | 3.4 |
| 1 | BA | 1008 | U | 3.4 |
| 35 | CO | 43 | GLU | 3.4 |
| 1 | BA | 1131 | G | 3.4 |
| 16 | BP | 63 | GLN | 3.4 |
| 22 | CA | 1465 | G | 3.4 |
| 29 | CH | 2 | GLN | 3.4 |
| 29 | DH | 42 | LYS | 3.4 |
| 46 | CZ | 38 | GLN | 3.4 |
| 22 | CA | 877 | A | 3.4 |
| 53 | DA | 2108 | A | 3.4 |
| 2 | BB | 110 | SER | 3.4 |
| 48 | D1 | 8 | PRO | 3.4 |
| 30 | DJ | 127 | ARG | 3.4 |
| 2 | AB | 88 | ASP | 3.4 |
| 24 | CC | 49 | ILE | 3.4 |
| 35 | CO | 52 | ILE | 3.4 |
| 1 | BA | 89 | U | 3.4 |
| 13 | BM | 59 | GLU | 3.4 |
| 17 | BQ | 80 | GLU | 3.4 |
| 22 | CA | 2833 | U | 3.4 |
| 33 | CM | 52 | GLY | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 34 | CN | 99 | GLY | 3.4 |
| 11 | AK | 59 | THR | 3.3 |
| 34 | CN | 24 | THR | 3.3 |
| 14 | BN | 71 | HIS | 3.3 |
| 1 | BA | 1039 | G | 3.3 |
| 7 | BG | 26 | PHE | 3.3 |
| 24 | DC | 216 | VAL | 3.3 |
| 29 | DH | 19 | VAL | 3.3 |
| 42 | DV | 49 | VAL | 3.3 |
| 29 | CH | 82 | SER | 3.3 |
| 24 | DC | 122 | ALA | 3.3 |
| 33 | CM | 119 | PRO | 3.3 |
| 2 | AB | 212 | LEU | 3.3 |
| 34 | CN | 112 | LEU | 3.3 |
| 39 | CS | 39 | LEU | 3.3 |
| 45 | DY | 22 | LEU | 3.3 |
| 1 | BA | 1023 | U | 3.3 |
| 10 | BJ | 14 | ASP | 3.3 |
| 19 | AS | 27 | ASP | 3.3 |
| 22 | CA | 545 | U | 3.3 |
| 26 | CE | 155 | GLU | 3.3 |
| 29 | DH | 109 | GLU | 3.3 |
| 40 | CT | 94 | ASP | 3.3 |
| 42 | CV | 88 | GLU | 3.3 |
| 44 | DX | 85 | GLU | 3.3 |
| 53 | DA | 355 | U | 3.3 |
| 14 | BN | 78 | GLY | 3.3 |
| 31 | CK | 82 | GLY | 3.3 |
| 40 | CT | 98 | LYS | 3.3 |
| 2 | AB | 213 | TYR | 3.3 |
| 39 | CS | 83 | TYR | 3.3 |
| 1 | BA | 1363 | A | 3.3 |
| 2 | BB | 9 | MET | 3.3 |
| 6 | AF | 102 | MET | 3.3 |
| 22 | CA | 1552 | A | 3.3 |
| 24 | CC | 146 | MET | 3.3 |
| 35 | DO | 1 | MET | 3.3 |
| 28 | CG | 152 | ARG | 3.3 |
| 35 | CO | 17 | ARG | 3.3 |
| 41 | CU | 12 | ARG | 3.3 |
| 21 | AU | 9 | ASN | 3.3 |
| 27 | CF | 121 | SER | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 53 | DA | 2159 | G | 3.3 |
| 8 | AH | 110 | VAL | 3.3 |
| 21 | AU | 32 | VAL | 3.3 |
| 2 | AB | 83 | ALA | 3.3 |
| 9 | AI | 120 | LYS | 3.3 |
| 20 | BT | 69 | LYS | 3.3 |
| 24 | DC | 210 | ALA | 3.3 |
| 55 | DI | 110 | ALA | 3.3 |
| 16 | BP | 49 | GLY | 3.3 |
| 37 | CQ | 12 | GLN | 3.3 |
| 46 | CZ | 62 | GLY | 3.3 |
| 1 | BA | 179 | A | 3.3 |
| 2 | AB | 21 | ARG | 3.3 |
| 16 | BP | 75 | ILE | 3.3 |
| 22 | CA | 1439 | A | 3.3 |
| 22 | CA | 2376 | A | 3.3 |
| 28 | CG | 163 | ARG | 3.3 |
| 40 | CT | 24 | ILE | 3.3 |
| 49 | C2 | 6 | ARG | 3.3 |
| 9 | BI | 13 | LYS | 3.3 |
| 10 | BJ | 11 | LYS | 3.3 |
| 10 | BJ | 30 | LYS | 3.3 |
| 22 | CA | 407 | G | 3.3 |
| 26 | CE | 116 | ASP | 3.3 |
| 37 | CQ | 14 | LYS | 3.3 |
| 42 | CV | 47 | LYS | 3.3 |
| 2 | BB | 34 | ALA | 3.3 |
| 3 | BC | 95 | ALA | 3.3 |
| 38 | CR | 4 | VAL | 3.3 |
| 48 | C1 | 2 | ALA | 3.3 |
| 22 | CA | 353 | C | 3.3 |
| 29 | DH | 120 | GLY | 3.3 |
| 8 | BH | 63 | LEU | 3.3 |
| 11 | AK | 42 | LEU | 3.3 |
| 3 | BC | 179 | ARG | 3.3 |
| 38 | CR | 28 | ARG | 3.3 |
| 3 | BC | 108 | LYS | 3.3 |
| 28 | CG | 138 | LYS | 3.3 |
| 24 | DC | 51 | THR | 3.3 |
| 25 | CD | 133 | THR | 3.3 |
| 31 | DK | 81 | ILE | 3.3 |
| 33 | DM | 103 | ILE | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 37 | DQ | 2 | SER | 3.3 |
| 38 | CR | 17 | ILE | 3.3 |
| 39 | CS | 19 | THR | 3.3 |
| 5 | AE | 160 | SER | 3.3 |
| 7 | AG | 9 | GLN | 3.3 |
| 22 | CA | 271 | G | 3.3 |
| 22 | CA | 1238 | G | 3.3 |
| 30 | DJ | 56 | PRO | 3.3 |
| 38 | CR | 45 | TYR | 3.3 |
| 2 | BB | 99 | GLY | 3.3 |
| 11 | AK | 99 | ALA | 3.3 |
| 2 | AB | 91 | PHE | 3.3 |
| 7 | AG | 141 | VAL | 3.3 |
| 7 | BG | 32 | VAL | 3.3 |
| 9 | BI | 11 | ARG | 3.3 |
| 15 | BO | 86 | GLY | 3.3 |
| 28 | CG | 100 | GLY | 3.3 |
| 29 | CH | 111 | ALA | 3.3 |
| 33 | DM | 37 | GLY | 3.3 |
| 41 | CU | 18 | GLU | 3.3 |
| 43 | CW | 16 | ALA | 3.3 |
| 43 | CW | 39 | ALA | 3.3 |
| 36 | CP | 92 | PHE | 3.3 |
| 39 | DS | 75 | VAL | 3.3 |
| 54 | DD | 127 | PHE | 3.3 |
| 55 | DI | 42 | ARG | 3.3 |
| 2 | BB | 112 | LYS | 3.3 |
| 43 | CW | 5 | ASN | 3.3 |
| 53 | DA | 1098 | A | 3.3 |
| 49 | C2 | 40 | ASP | 3.3 |
| 2 | BB | 72 | THR | 3.3 |
| 7 | BG | 38 | THR | 3.3 |
| 9 | BI | 88 | MET | 3.3 |
| 26 | CE | 107 | SER | 3.3 |
| 33 | CM | 42 | SER | 3.3 |
| 40 | CT | 15 | GLN | 3.3 |
| 21 | AU | 11 | PRO | 3.3 |
| 22 | CA | 183 | C | 3.3 |
| 40 | CT | 85 | ILE | 3.3 |
| 22 | CA | 1475 | G | 3.3 |
| 3 | AC | 107 | ARG | 3.3 |
| 11 | BK | 53 | ARG | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 11 | AK | 75 | LYS | 3.3 |
| 28 | DG | 177 | LYS | 3.3 |
| 33 | CM | 31 | GLY | 3.3 |
| 11 | BK | 67 | ALA | 3.3 |
| 25 | CD | 102 | ALA | 3.3 |
| 22 | CA | 38 | A | 3.3 |
| 32 | CL | 13 | ASN | 3.3 |
| 2 | AB | 4 | VAL | 3.3 |
| 14 | BN | 77 | PHE | 3.3 |
| 22 | CA | 1466 | U | 3.3 |
| 21 | BU | 16 | LEU | 3.3 |
| 7 | BG | 41 | SER | 3.3 |
| 10 | BJ | 47 | GLU | 3.3 |
| 16 | AP | 44 | SER | 3.3 |
| 29 | CH | 109 | GLU | 3.3 |
| 7 | AG | 38 | THR | 3.3 |
| 41 | CU | 33 | LYS | 3.2 |
| 42 | DV | 50 | PRO | 3.3 |
| 43 | CW | 46 | LYS | 3.2 |
| 1 | BA | 275 | G | 3.2 |
| 1 | BA | 1439 | G | 3.2 |
| 22 | CA | 2286 | G | 3.2 |
| 52 | C5 | 38 | GLY | 3.2 |
| 1 | BA | 1311 | A | 3.2 |
| 37 | CQ | 42 | ALA | 3.2 |
| 14 | AN | 11 | VAL | 3.2 |
| 7 | BG | 96 | ARG | 3.2 |
| 14 | BN | 63 | ARG | 3.2 |
| 27 | CF | 61 | SER | 3.2 |
| 44 | CX | 35 | SER | 3.2 |
| 54 | DD | 145 | SER | 3.2 |
| 35 | CO | 20 | MET | 3.2 |
| 1 | BA | 91 | U | 3.2 |
| 31 | CK | 110 | PRO | 3.2 |
| 1 | BA | 76 | G | 3.2 |
| 25 | CD | 44 | GLY | 3.2 |
| 24 | CC | 121 | ASP | 3.2 |
| 2 | BB | 140 | GLU | 3.2 |
| 22 | CA | 1596 | A | 3.2 |
| 43 | CW | 24 | ASN | 3.2 |
| 41 | CU | 25 | GLU | 3.2 |
| 42 | CV | 66 | GLN | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 48 | C1 | 19 | HIS | 3.2 |
| 53 | DA | 278 | A | 3.2 |
| 3 | BC | 120 | ILE | 3.2 |
| 6 | BF | 83 | ALA | 3.2 |
| 35 | CO | 61 | ALA | 3.2 |
| 41 | CU | 41 | ALA | 3.2 |
| 27 | DF | 72 | LYS | 3.2 |
| 12 | BL | 56 | ARG | 3.2 |
| 9 | BI | 15 | SER | 3.2 |
| 34 | CN | 27 | SER | 3.2 |
| 53 | DA | 1729 | U | 3.2 |
| 53 | DA | 2106 | U | 3.2 |
| 26 | CE | 85 | PHE | 3.2 |
| 31 | CK | 92 | MET | 3.2 |
| 2 | AB | 20 | THR | 3.2 |
| 32 | CL | 120 | PRO | 3.2 |
| 29 | DH | 122 | LEU | 3.2 |
| 51 | D4 | 6 | THR | 3.2 |
| 2 | BB | 149 | GLY | 3.2 |
| 24 | CC | 119 | GLY | 3.2 |
| 50 | C3 | 13 | ASN | 3.2 |
| 1 | BA | 75 | G | 3.2 |
| 1 | BA | 838 | G | 3.2 |
| 22 | CA | 600 | G | 3.2 |
| 22 | CA | 1719 | G | 3.2 |
| 22 | CA | 2410 | G | 3.2 |
| 25 | CD | 134 | HIS | 3.2 |
| 3 | AC | 79 | LYS | 3.2 |
| 13 | BM | 107 | ARG | 3.2 |
| 16 | BP | 51 | ARG | 3.2 |
| 24 | CC | 48 | ARG | 3.2 |
| 53 | DA | 2118 | U | 3.2 |
| 2 | AB | 200 | ILE | 3.2 |
| 51 | D4 | 61 | CYS | 3.2 |
| 29 | CH | 55 | GLU | 3.2 |
| 37 | DQ | 98 | TYR | 3.2 |
| 6 | BF | 72 | ASP | 3.2 |
| 29 | CH | 18 | GLN | 3.2 |
| 34 | CN | 25 | ASP | 3.2 |
| 42 | CV | 81 | ASP | 3.2 |
| 5 | BE | 137 | VAL | 3.2 |
| 6 | BF | 97 | THR | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 8 | BH | 51 | VAL | 3.2 |
| 9 | AI | 116 | VAL | 3.2 |
| 43 | CW | 62 | THR | 3.2 |
| 1 | AA | 843 | U | 3.2 |
| 2 | BB | 162 | PHE | 3.2 |
| 54 | DD | 153 | GLY | 3.2 |
| 51 | D4 | 62 | LEU | 3.2 |
| 53 | DA | 1871 | A | 3.2 |
| 53 | DA | 2155 | U | 3.2 |
| 22 | CA | 1450 | G | 3.2 |
| 22 | CA | 1456 | G | 3.2 |
| 22 | CA | 1540 | G | 3.2 |
| 22 | CA | 274 | C | 3.2 |
| 22 | CA | 2306 | C | 3.2 |
| 3 | BC | 133 | ALA | 3.2 |
| 29 | CH | 53 | GLU | 3.2 |
| 31 | CK | 98 | GLU | 3.2 |
| 8 | BH | 5 | ASP | 3.2 |
| 19 | BS | 6 | LYS | 3.2 |
| 20 | BT | 44 | LYS | 3.2 |
| 51 | C4 | 5 | LYS | 3.2 |
| 3 | BC | 142 | MET | 3.2 |
| 10 | AJ | 33 | GLY | 3.2 |
| 24 | CC | 161 | TYR | 3.2 |
| 29 | CH | 1 | MET | 3.2 |
| 38 | DR | 24 | TYR | 3.2 |
| 22 | CA | 1385 | A | 3.2 |
| 32 | CL | 30 | ARG | 3.2 |
| 35 | CO | 37 | THR | 3.2 |
| 53 | DA | 1847 | A | 3.2 |
| 5 | BE | 112 | ARG | 3.2 |
| 35 | CO | 118 | ARG | 3.2 |
| 5 | AE | 123 | VAL | 3.2 |
| 14 | BN | 45 | VAL | 3.2 |
| 24 | CC | 165 | VAL | 3.2 |
| 1 | BA | 847 | G | 3.2 |
| 9 | AI | 118 | LEU | 3.2 |
| 22 | CA | 1079 | C | 3.2 |
| 33 | DM | 61 | LEU | 3.2 |
| 46 | CZ | 13 | GLU | 3.2 |
| 2 | BB | 152 | LYS | 3.2 |
| 25 | CD | 162 | ALA | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 29 | CH | 39 | ALA | 3.2 |
| 30 | DJ | 72 | LYS | 3.2 |
| 34 | CN | 100 | LYS | 3.2 |
| 35 | DO | 14 | SER | 3.2 |
| 38 | CR | 59 | GLN | 3.2 |
| 39 | CS | 3 | ALA | 3.2 |
| 42 | CV | 46 | GLN | 3.2 |
| 51 | C4 | 10 | ALA | 3.2 |
| 55 | DI | 29 | ASP | 3.2 |
| 2 | BB | 146 | ASN | 3.2 |
| 9 | AI | 79 | ILE | 3.2 |
| 45 | CY | 64 | ILE | 3.2 |
| 1 | BA | 978 | A | 3.2 |
| 6 | BF | 21 | MET | 3.2 |
| 22 | CA | 2211 | A | 3.2 |
| 31 | CK | 13 | ARG | 3.2 |
| 33 | CM | 33 | ARG | 3.2 |
| 46 | CZ | 7 | ARG | 3.2 |
| 29 | CH | 128 | HIS | 3.2 |
| 1 | BA | 840 | C | 3.2 |
| 22 | CA | 1072 | C | 3.2 |
| 22 | CA | 1726 | C | 3.2 |
| 25 | CD | 61 | THR | 3.2 |
| 26 | CE | 43 | THR | 3.2 |
| 34 | CN | 129 | THR | 3.2 |
| 39 | DS | 83 | TYR | 3.2 |
| 13 | AM | 60 | VAL | 3.2 |
| 29 | DH | 103 | VAL | 3.2 |
| 29 | CH | 35 | LYS | 3.2 |
| 31 | CK | 85 | LYS | 3.2 |
| 47 | C0 | 17 | LEU | 3.2 |
| 55 | DI | 95 | LEU | 3.2 |
| 2 | BB | 167 | ASP | 3.1 |
| 31 | CK | 120 | ARG | 3.1 |
| 40 | DT | 110 | ARG | 3.1 |
| 42 | CV | 94 | ARG | 3.1 |
| 49 | C2 | 28 | ARG | 3.1 |
| 1 | BA | 1044 | A | 3.1 |
| 1 | BA | 1269 | A | 3.1 |
| 9 | AI | 23 | PRO | 3.1 |
| 24 | CC | 179 | GLY | 3.1 |
| 24 | DC | 215 | GLY | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 35 | CO | 7 | GLY | 3.1 |
| 22 | CA | 1173 | U | 3.1 |
| 38 | DR | 9 | ILE | 3.1 |
| 54 | DD | 140 | HIS | 3.1 |
| 2 | BB | 119 | THR | 3.1 |
| 13 | AM | 78 | LYS | 3.1 |
| 16 | AP | 80 | LYS | 3.1 |
| 50 | C3 | 43 | THR | 3.1 |
| 2 | AB | 153 | ASP | 3.1 |
| 17 | BQ | 53 | CYS | 3.1 |
| 17 | BQ | 64 | CYS | 3.1 |
| 1 | BA | 954 | G | 3.1 |
| 22 | CA | 1279 | G | 3.1 |
| 8 | BH | 104 | VAL | 3.1 |
| 11 | AK | 129 | VAL | 3.1 |
| 26 | DE | 52 | VAL | 3.1 |
| 38 | CR | 31 | VAL | 3.1 |
| 7 | AG | 62 | PHE | 3.1 |
| 16 | BP | 40 | ASN | 3.1 |
| 20 | BT | 66 | LEU | 3.1 |
| 24 | CC | 174 | LEU | 3.1 |
| 25 | CD | 21 | SER | 3.1 |
| 28 | DG | 105 | LEU | 3.1 |
| 29 | CH | 5 | LEU | 3.1 |
| 30 | DJ | 11 | LEU | 3.1 |
| 34 | CN | 95 | LEU | 3.1 |
| 34 | DN | 59 | ARG | 3.1 |
| 35 | DO | 10 | LEU | 3.1 |
| 37 | CQ | 39 | ARG | 3.1 |
| 41 | CU | 93 | LEU | 3.1 |
| 45 | CY | 16 | ASN | 3.1 |
| 7 | AG | 152 | ALA | 3.1 |
| 22 | CA | 866 | A | 3.1 |
| 22 | CA | 1070 | A | 3.1 |
| 22 | CA | 1508 | A | 3.1 |
| 23 | CB | 59 | A | 3.1 |
| 38 | DR | 10 | ALA | 3.1 |
| 53 | DA | 1094 | U | 3.1 |
| 55 | DI | 112 | ALA | 3.1 |
| 3 | BC | 13 | GLY | 3.1 |
| 11 | AK | 39 | GLY | 3.1 |
| 24 | DC | 55 | GLY | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 31 | CK | 111 | LYS | 3.1 |
| 2 | BB | 154 | MET | 3.1 |
| 26 | DE | 9 | GLN | 3.1 |
| 9 | BI | 30 | ILE | 3.1 |
| 18 | AR | 28 | THR | 3.1 |
| 3 | BC | 169 | ARG | 3.1 |
| 13 | AM | 92 | ARG | 3.1 |
| 15 | BO | 6 | GLU | 3.1 |
| 20 | BT | 29 | ARG | 3.1 |
| 33 | CM | 86 | GLU | 3.1 |
| 1 | AA | 4 | U | 3.1 |
| 1 | BA | 209 | U | 3.1 |
| 1 | BA | 1297 | G | 3.1 |
| 21 | BU | 51 | SER | 3.1 |
| 22 | CA | 365 | U | 3.1 |
| 22 | CA | 585 | G | 3.1 |
| 38 | DR | 25 | TYR | 3.1 |
| 53 | DA | 284 | U | 3.1 |
| 53 | DA | 2049 | G | 3.1 |
| 53 | DA | 2144 | G | 3.1 |
| 3 | BC | 106 | VAL | 3.1 |
| 10 | BJ | 51 | VAL | 3.1 |
| 11 | AK | 84 | VAL | 3.1 |
| 28 | CG | 134 | LYS | 3.1 |
| 40 | CT | 71 | VAL | 3.1 |
| 1 | BA | 77 | A | 3.1 |
| 1 | BA | 974 | A | 3.1 |
| 10 | BJ | 73 | LEU | 3.1 |
| 22 | CA | 213 | A | 3.1 |
| 22 | CA | 1505 | A | 3.1 |
| 22 | CA | 1507 | C | 3.1 |
| 29 | DH | 54 | LEU | 3.1 |
| 6 | AF | 95 | ALA | 3.1 |
| 29 | CH | 102 | ALA | 3.1 |
| 30 | DJ | 16 | GLY | 3.1 |
| 30 | DJ | 26 | PRO | 3.1 |
| 40 | CT | 56 | ALA | 3.1 |
| 3 | BC | 36 | ASP | 3.1 |
| 1 | BA | 1295 | U | 3.1 |
| 8 | BH | 91 | GLU | 3.1 |
| 14 | BN | 65 | ARG | 3.1 |
| 14 | BN | 100 | SER | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 33 | CM | 109 | LYS | 3.1 |
| 34 | CN | 58 | LYS | 3.1 |
| 54 | DD | 137 | SER | 3.1 |
| 22 | CA | 488 | G | 3.1 |
| 22 | CA | 1448 | G | 3.1 |
| 22 | CA | 2141 | G | 3.1 |
| 53 | DA | 287 | G | 3.1 |
| 22 | CA | 1413 | A | 3.1 |
| 9 | BI | 29 | VAL | 3.1 |
| 38 | CR | 82 | GLY | 3.1 |
| 44 | CX | 23 | VAL | 3.1 |
| 24 | CC | 210 | ALA | 3.1 |
| 24 | DC | 154 | LEU | 3.1 |
| 33 | CM | 10 | GLU | 3.1 |
| 41 | CU | 56 | GLU | 3.1 |
| 47 | C0 | 29 | LEU | 3.1 |
| 24 | CC | 240 | PHE | 3.1 |
| 35 | CO | 21 | PHE | 3.1 |
| 47 | C0 | 53 | PHE | 3.1 |
| 13 | AM | 79 | ARG | 3.1 |
| 7 | BG | 110 | LYS | 3.1 |
| 15 | BO | 20 | ASN | 3.1 |
| 43 | CW | 49 | ASN | 3.1 |
| 44 | CX | 19 | LYS | 3.1 |
| 49 | C2 | 22 | THR | 3.1 |
| 1 | BA | 1140 | C | 3.1 |
| 1 | AA | 203 | G | 3.1 |
| 1 | BA | 941 | G | 3.1 |
| 15 | BO | 36 | ILE | 3.1 |
| 17 | BQ | 25 | ILE | 3.1 |
| 1 | BA | 992 | U | 3.1 |
| 22 | CA | 45 | G | 3.1 |
| 22 | CA | 437 | U | 3.1 |
| 22 | CA | 1429 | G | 3.1 |
| 22 | CA | 2144 | G | 3.1 |
| 22 | CA | 2190 | G | 3.1 |
| 41 | CU | 30 | ILE | 3.1 |
| 29 | DH | 60 | GLU | 3.1 |
| 35 | CO | 82 | GLU | 3.1 |
| 53 | DA | 286 | U | 3.1 |
| 16 | BP | 64 | GLY | 3.1 |
| 20 | BT | 20 | HIS | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 42 | CV | 57 | GLY | 3.1 |
| 51 | C4 | 43 | HIS | 3.1 |
| 3 | BC | 112 | ASP | 3.1 |
| 5 | BE | 150 | PRO | 3.1 |
| 40 | CT | 80 | PRO | 3.1 |
| 26 | CE | 101 | TYR | 3.1 |
| 34 | CN | 103 | TYR | 3.1 |
| 54 | DD | 141 | ARG | 3.1 |
| 55 | DI | 61 | ARG | 3.1 |
| 6 | BF | 35 | LYS | 3.1 |
| 24 | DC | 190 | ALA | 3.1 |
| 44 | CX | 21 | LEU | 3.1 |
| 1 | AA | 1028 | C | 3.1 |
| 1 | BA | 88 | U | 3.1 |
| 1 | BA | 723 | U | 3.1 |
| 2 | BB | 223 | GLU | 3.1 |
| 20 | BT | 15 | GLU | 3.1 |
| 22 | CA | 937 | C | 3.1 |
| 26 | DE | 53 | THR | 3.1 |
| 9 | AI | 5 | GLN | 3.1 |
| 22 | CA | 340 | A | 3.1 |
| 22 | CA | 1321 | A | 3.1 |
| 39 | CS | 23 | GLU | 3.1 |
| 46 | CZ | 25 | GLN | 3.1 |
| 9 | AI | 56 | ASP | 3.1 |
| 11 | BK | 48 | GLY | 3.1 |
| 20 | BT | 68 | HIS | 3.1 |
| 33 | CM | 49 | GLY | 3.1 |
| 39 | CS | 8 | GLY | 3.1 |
| 45 | CY | 11 | ARG | 3.1 |
| 55 | DI | 36 | ASP | 3.1 |
| 2 | BB | 29 | PRO | 3.1 |
| 2 | BB | 61 | ALA | 3.0 |
| 3 | AC | 113 | ALA | 3.0 |
| 3 | BC | 25 | ASN | 3.0 |
| 5 | BE | 122 | ASN | 3.0 |
| 26 | CE | 192 | ALA | 3.0 |
| 3 | BC | 97 | VAL | 3.0 |
| 11 | BK | 100 | LEU | 3.0 |
| 21 | BU | 6 | VAL | 3.0 |
| 26 | CE | 52 | VAL | 3.0 |
| 30 | DJ | 17 | MET | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 35 | CO | 115 | LEU | 3.0 |
| 22 | CA | 184 | C | 3.0 |
| 7 | AG | 57 | SER | 3.0 |
| 32 | CL | 14 | SER | 3.0 |
| 44 | CX | 69 | PHE | 3.0 |
| 4 | AD | 73 | ARG | 3.0 |
| 40 | CT | 7 | HIS | 3.0 |
| 22 | CA | 1517 | G | 3.0 |
| 22 | CA | 1857 | G | 3.0 |
| 1 | BA | 472 | U | 3.0 |
| 1 | BA | 991 | U | 3.0 |
| 9 | BI | 125 | PRO | 3.0 |
| 28 | DG | 48 | ASN | 3.0 |
| 2 | BB | 209 | ALA | 3.0 |
| 25 | CD | 132 | ALA | 3.0 |
| 33 | CM | 72 | ALA | 3.0 |
| 39 | CS | 42 | ALA | 3.0 |
| 33 | DM | 55 | MET | 3.0 |
| 2 | AB | 54 | LEU | 3.0 |
| 2 | AB | 92 | VAL | 3.0 |
| 7 | BG | 136 | LYS | 3.0 |
| 22 | CA | 1080 | A | 3.0 |
| 22 | CA | 1713 | A | 3.0 |
| 35 | CO | 14 | SER | 3.0 |
| 38 | CR | 41 | LYS | 3.0 |
| 41 | CU | 31 | VAL | 3.0 |
| 49 | C2 | 10 | LYS | 3.0 |
| 20 | BT | 10 | ARG | 3.0 |
| 42 | CV | 15 | THR | 3.0 |
| 3 | BC | 6 | HIS | 3.0 |
| 24 | CC | 233 | GLY | 3.0 |
| 24 | DC | 47 | GLY | 3.0 |
| 31 | DK | 115 | GLY | 3.0 |
| 2 | BB | 169 | GLU | 3.0 |
| 10 | BJ | 78 | GLU | 3.0 |
| 53 | DA | 1177 | G | 3.0 |
| 55 | DI | 17 | GLU | 3.0 |
| 2 | BB | 87 | CYS | 3.0 |
| 7 | AG | 14 | PRO | 3.0 |
| 1 | BA | 1141 | C | 3.0 |
| 22 | CA | 2295 | C | 3.0 |
| 22 | CA | 2666 | C | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 11 | BK | 110 | ILE | 3.0 |
| 24 | CC | 54 | ILE | 3.0 |
| 39 | CS | 48 | LYS | 3.0 |
| 2 | AB | 209 | ALA | 3.0 |
| 5 | AE | 93 | ARG | 3.0 |
| 24 | CC | 2 | ALA | 3.0 |
| 26 | CE | 87 | ALA | 3.0 |
| 29 | CH | 100 | ALA | 3.0 |
| 33 | CM | 133 | ALA | 3.0 |
| 14 | AN | 32 | SER | 3.0 |
| 22 | CA | 431 | U | 3.0 |
| 22 | CA | 1528 | A | 3.0 |
| 22 | CA | 1749 | A | 3.0 |
| 39 | CS | 40 | MET | 3.0 |
| 2 | BB | 147 | SER | 3.0 |
| 43 | CW | 66 | ASP | 3.0 |
| 53 | DA | 2130 | U | 3.0 |
| 3 | AC | 106 | VAL | 3.0 |
| 14 | AN | 96 | LEU | 3.0 |
| 24 | CC | 252 | THR | 3.0 |
| 24 | DC | 195 | VAL | 3.0 |
| 38 | DR | 45 | TYR | 3.0 |
| 55 | DI | 23 | LEU | 3.0 |
| 11 | AK | 43 | GLY | 3.0 |
| 33 | DM | 49 | GLY | 3.0 |
| 45 | CY | 17 | ASN | 3.0 |
| 42 | CV | 54 | GLN | 3.0 |
| 46 | CZ | 39 | GLN | 3.0 |
| 1 | AA | 1011 | C | 3.0 |
| 22 | CA | 1504 | A | 3.0 |
| 42 | CV | 89 | ASP | 3.0 |
| 48 | C1 | 31 | ASP | 3.0 |
| 53 | DA | 1090 | A | 3.0 |
| 7 | AG | 39 | ALA | 3.0 |
| 7 | BG | 106 | GLU | 3.0 |
| 10 | AJ | 94 | ALA | 3.0 |
| 24 | CC | 272 | SER | 3.0 |
| 29 | DH | 82 | SER | 3.0 |
| 36 | CP | 5 | SER | 3.0 |
| 44 | DX | 84 | ALA | 3.0 |
| 3 | BC | 14 | ILE | 3.0 |
| 11 | AK | 107 | ILE | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 21 | BU | 4 | ILE | 3.0 |
| 31 | CK | 84 | ILE | 3.0 |
| 52 | C5 | 26 | ILE | 3.0 |
| 3 | BC | 81 | GLY | 3.0 |
| 3 | BC | 205 | GLY | 3.0 |
| 11 | BK | 43 | GLY | 3.0 |
| 26 | CE | 54 | GLY | 3.0 |
| 3 | AC | 43 | LEU | 3.0 |
| 3 | BC | 76 | VAL | 3.0 |
| 15 | BO | 70 | LEU | 3.0 |
| 16 | BP | 46 | LYS | 3.0 |
| 37 | CQ | 97 | LEU | 3.0 |
| 49 | C2 | 11 | LEU | 3.0 |
| 22 | CA | 1458 | U | 3.0 |
| 22 | CA | 2187 | U | 3.0 |
| 25 | CD | 143 | PRO | 3.0 |
| 43 | CW | 37 | PRO | 3.0 |
| 22 | CA | 647 | G | 3.0 |
| 33 | CM | 48 | ARG | 3.0 |
| 38 | CR | 92 | ARG | 3.0 |
| 4 | BD | 166 | GLU | 3.0 |
| 16 | AP | 48 | GLU | 3.0 |
| 43 | CW | 45 | ASP | 3.0 |
| 53 | DA | 2119 | A | 3.0 |
| 2 | BB | 160 | ALA | 3.0 |
| 20 | BT | 5 | LYS | 3.0 |
| 3 | BC | 159 | GLY | 3.0 |
| 5 | AE | 122 | ASN | 3.0 |
| 25 | CD | 94 | GLN | 3.0 |
| 29 | CH | 4 | ILE | 3.0 |
| 38 | CR | 74 | ILE | 3.0 |
| 15 | BO | 17 | ARG | 3.0 |
| 2 | AB | 201 | PRO | 3.0 |
| 4 | BD | 68 | LEU | 3.0 |
| 7 | BG | 89 | VAL | 3.0 |
| 11 | BK | 86 | VAL | 3.0 |
| 15 | BO | 27 | VAL | 3.0 |
| 29 | CH | 118 | PRO | 3.0 |
| 29 | DH | 70 | GLU | 3.0 |
| 32 | CL | 8 | LEU | 3.0 |
| 38 | DR | 31 | VAL | 3.0 |
| 22 | CA | 220 | G | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | CA | 1449 | G | 3.0 |
| 33 | DM | 64 | PHE | 3.0 |
| 3 | AC | 62 | LYS | 3.0 |
| 38 | CR | 112 | LYS | 3.0 |
| 48 | C1 | 12 | LYS | 3.0 |
| 34 | CN | 97 | GLN | 3.0 |
| 38 | CR | 68 | ALA | 3.0 |
| 2 | AB | 56 | GLU | 2.9 |
| 3 | BC | 161 | GLU | 2.9 |
| 33 | DM | 22 | GLY | 2.9 |
| 53 | DA | 2150 | C | 2.9 |
| 55 | DI | 46 | ARG | 2.9 |
| 47 | D0 | 32 | ILE | 2.9 |
| 19 | AS | 12 | ASP | 2.9 |
| 52 | C5 | 14 | CYS | 2.9 |
| 44 | CX | 74 | PRO | 2.9 |
| 1 | BA | 1272 | G | 2.9 |
| 22 | CA | 2156 | G | 2.9 |
| 22 | CA | 2837 | A | 2.9 |
| 23 | CB | 16 | G | 2.9 |
| 25 | CD | 24 | VAL | 2.9 |
| 29 | DH | 115 | VAL | 2.9 |
| 31 | CK | 12 | LYS | 2.9 |
| 31 | CK | 140 | LEU | 2.9 |
| 51 | C4 | 25 | LYS | 2.9 |
| 53 | DA | 1093 | G | 2.9 |
| 53 | DA | 2688 | G | 2.9 |
| 24 | CC | 103 | TYR | 2.9 |
| 38 | CR | 25 | TYR | 2.9 |
| 26 | CE | 75 | SER | 2.9 |
| 36 | CP | 95 | SER | 2.9 |
| 6 | AF | 80 | PHE | 2.9 |
| 7 | BG | 67 | GLU | 2.9 |
| 24 | CC | 82 | GLU | 2.9 |
| 35 | DO | 13 | ASN | 2.9 |
| 17 | BQ | 77 | ARG | 2.9 |
| 26 | CE | 79 | ARG | 2.9 |
| 7 | BG | 24 | ALA | 2.9 |
| 16 | BP | 43 | ALA | 2.9 |
| 25 | CD | 53 | GLY | 2.9 |
| 25 | CD | 75 | ALA | 2.9 |
| 26 | CE | 86 | ALA | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 29 | DH | 111 | ALA | 2.9 |
| 33 | CM | 20 | GLY | 2.9 |
| 33 | CM | 131 | ALA | 2.9 |
| 38 | CR | 86 | ALA | 2.9 |
| 50 | C3 | 40 | ALA | 2.9 |
| 52 | C5 | 29 | ALA | 2.9 |
| 1 | AA | 209 | U | 2.9 |
| 2 | AB | 193 | PRO | 2.9 |
| 10 | BJ | 46 | LYS | 2.9 |
| 11 | BK | 111 | THR | 2.9 |
| 27 | DF | 78 | LYS | 2.9 |
| 17 | AQ | 61 | ILE | 2.9 |
| 41 | CU | 48 | GLN | 2.9 |
| 1 | BA | 1221 | G | 2.9 |
| 4 | BD | 171 | LEU | 2.9 |
| 53 | DA | 1653 | G | 2.9 |
| 3 | AC | 151 | VAL | 2.9 |
| 7 | AG | 92 | ARG | 2.9 |
| 13 | AM | 30 | SER | 2.9 |
| 14 | BN | 80 | SER | 2.9 |
| 20 | BT | 26 | SER | 2.9 |
| 24 | DC | 204 | VAL | 2.9 |
| 28 | CG | 38 | ASN | 2.9 |
| 1 | BA | 1218 | C | 2.9 |
| 37 | CQ | 99 | TYR | 2.9 |
| 16 | BP | 62 | GLY | 2.9 |
| 21 | AU | 13 | ASP | 2.9 |
| 31 | CK | 60 | ASP | 2.9 |
| 32 | CL | 33 | ALA | 2.9 |
| 40 | CT | 58 | ALA | 2.9 |
| 40 | DT | 89 | ALA | 2.9 |
| 54 | DD | 162 | ALA | 2.9 |
| 55 | DI | 44 | ALA | 2.9 |
| 1 | BA | 1261 | A | 2.9 |
| 4 | AD | 30 | THR | 2.9 |
| 6 | BF | 46 | GLN | 2.9 |
| 22 | CA | 666 | A | 2.9 |
| 25 | CD | 23 | PRO | 2.9 |
| 26 | CE | 89 | PRO | 2.9 |
| 31 | CK | 50 | THR | 2.9 |
| 29 | CH | 44 | ILE | 2.9 |
| 33 | CM | 111 | ILE | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 47 | C0 | 5 | ILE | 2.9 |
| 1 | AA | 1034 | G | 2.9 |
| 22 | CA | 284 | U | 2.9 |
| 22 | CA | 1454 | C | 2.9 |
| 22 | CA | 2318 | G | 2.9 |
| 53 | DA | 276 | U | 2.9 |
| 53 | DA | 1100 | C | 2.9 |
| 53 | DA | 2035 | G | 2.9 |
| 5 | BE | 88 | VAL | 2.9 |
| 8 | BH | 31 | LYS | 2.9 |
| 9 | AI | 100 | LYS | 2.9 |
| 24 | CC | 202 | LEU | 2.9 |
| 11 | AK | 16 | VAL | 2.9 |
| 12 | BL | 87 | VAL | 2.9 |
| 26 | CE | 96 | VAL | 2.9 |
| 28 | CG | 15 | VAL | 2.9 |
| 28 | CG | 27 | LYS | 2.9 |
| 29 | CH | 146 | VAL | 2.9 |
| 42 | CV | 34 | VAL | 2.9 |
| 52 | C5 | 9 | LYS | 2.9 |
| 20 | AT | 43 | ASP | 2.9 |
| 11 | BK | 54 | GLY | 2.9 |
| 24 | DC | 161 | TYR | 2.9 |
| 29 | CH | 25 | TYR | 2.9 |
| 5 | AE | 10 | GLU | 2.9 |
| 26 | DE | 11 | ALA | 2.9 |
| 43 | CW | 12 | GLN | 2.9 |
| 9 | AI | 43 | THR | 2.9 |
| 9 | AI | 51 | PRO | 2.9 |
| 22 | CA | 231 | A | 2.9 |
| 22 | CA | 270 | A | 2.9 |
| 22 | CA | 614 | A | 2.9 |
| 22 | CA | 1509 | A | 2.9 |
| 5 | BE | 69 | ARG | 2.9 |
| 17 | BQ | 6 | ARG | 2.9 |
| 22 | CA | 1487 | U | 2.9 |
| 24 | CC | 9 | THR | 2.9 |
| 24 | CC | 219 | THR | 2.9 |
| 33 | CM | 2 | ARG | 2.9 |
| 12 | AL | 73 | ASN | 2.9 |
| 14 | BN | 62 | ASN | 2.9 |
| 48 | D1 | 6 | ASN | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 4 | BD | 148 | LYS | 2.9 |
| 22 | CA | 1462 | C | 2.9 |
| 22 | CA | 2422 | C | 2.9 |
| 33 | CM | 29 | LYS | 2.9 |
| 1 | BA | 148 | G | 2.9 |
| 1 | BA | 165 | G | 2.9 |
| 8 | BH | 125 | ILE | 2.9 |
| 13 | AM | 45 | ILE | 2.9 |
| 20 | AT | 4 | ILE | 2.9 |
| 25 | CD | 18 | ASP | 2.9 |
| 51 | C4 | 32 | ILE | 2.9 |
| 11 | BK | 82 | LEU | 2.9 |
| 20 | AT | 86 | LEU | 2.9 |
| 24 | CC | 24 | LEU | 2.9 |
| 28 | CG | 89 | LEU | 2.9 |
| 35 | DO | 20 | MET | 2.9 |
| 40 | CT | 26 | GLY | 2.9 |
| 40 | DT | 97 | LEU | 2.9 |
| 2 | AB | 19 | GLN | 2.9 |
| 25 | CD | 170 | VAL | 2.9 |
| 38 | DR | 61 | TRP | 2.9 |
| 54 | DD | 172 | VAL | 2.9 |
| 1 | BA | 467 | U | 2.9 |
| 22 | CA | 286 | U | 2.9 |
| 2 | AB | 219 | ALA | 2.9 |
| 15 | BO | 9 | ALA | 2.9 |
| 18 | BR | 62 | ALA | 2.9 |
| 20 | BT | 45 | ALA | 2.9 |
| 22 | CA | 1847 | A | 2.9 |
| 25 | CD | 77 | ARG | 2.9 |
| 55 | DI | 93 | ALA | 2.9 |
| 2 | BB | 42 | ASN | 2.9 |
| 3 | BC | 45 | LYS | 2.9 |
| 8 | AH | 49 | PHE | 2.9 |
| 13 | BM | 103 | LYS | 2.9 |
| 33 | CM | 70 | LYS | 2.9 |
| 33 | CM | 94 | THR | 2.9 |
| 37 | CQ | 37 | LYS | 2.9 |
| 23 | CB | 36 | C | 2.9 |
| 40 | CT | 104 | THR | 2.9 |
| 45 | CY | 25 | THR | 2.9 |
| 54 | DD | 136 | ASN | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | AI | 36 | GLU | 2.9 |
| 26 | CE | 197 | GLU | 2.9 |
| 39 | DS | 82 | HIS | 2.9 |
| 5 | BE | 102 | GLY | 2.9 |
| 22 | CA | 894 | U | 2.9 |
| 53 | DA | 2048 | G | 2.9 |
| 38 | DR | 26 | GLY | 2.9 |
| 39 | CS | 6 | GLN | 2.9 |
| 2 | AB | 27 | MET | 2.9 |
| 10 | AJ | 8 | ILE | 2.9 |
| 38 | DR | 17 | ILE | 2.9 |
| 1 | BA | 949 | A | 2.9 |
| 22 | CA | 352 | A | 2.9 |
| 29 | CH | 112 | LYS | 2.9 |
| 43 | CW | 25 | LYS | 2.9 |
| 5 | BE | 25 | VAL | 2.9 |
| 24 | CC | 220 | VAL | 2.9 |
| 24 | DC | 137 | VAL | 2.9 |
| 25 | CD | 122 | VAL | 2.9 |
| 27 | DF | 45 | ALA | 2.9 |
| 27 | DF | 75 | ALA | 2.9 |
| 29 | DH | 119 | ASN | 2.9 |
| 37 | CQ | 22 | PRO | 2.9 |
| 52 | C5 | 5 | ALA | 2.9 |
| 4 | AD | 170 | TRP | 2.9 |
| 19 | AS | 34 | TRP | 2.9 |
| 11 | AK | 105 | PHE | 2.8 |
| 22 | CA | 1058 | U | 2.8 |
| 25 | CD | 137 | SER | 2.8 |
| 33 | DM | 40 | SER | 2.8 |
| 39 | CS | 53 | PHE | 2.8 |
| 39 | DS | 77 | PHE | 2.8 |
| 31 | CK | 86 | GLN | 2.8 |
| 3 | AC | 74 | GLY | 2.8 |
| 33 | DM | 43 | GLY | 2.8 |
| 26 | CE | 123 | LYS | 2.8 |
| 40 | CT | 28 | LYS | 2.8 |
| 40 | CT | 73 | LYS | 2.8 |
| 1 | AA | 71 | A | 2.8 |
| 22 | CA | 2872 | A | 2.8 |
| 53 | DA | 1095 | A | 2.8 |
| 3 | BC | 57 | ILE | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 17 | BQ | 5 | ILE | 2.8 |
| 1 | AA | 999 | C | 2.8 |
| 19 | AS | 31 | LEU | 2.8 |
| 22 | CA | 1104 | C | 2.8 |
| 22 | CA | 2161 | C | 2.8 |
| 24 | CC | 95 | LEU | 2.8 |
| 43 | CW | 41 | GLU | 2.8 |
| 44 | DX | 21 | LEU | 2.8 |
| 2 | BB | 70 | VAL | 2.8 |
| 4 | BD | 61 | VAL | 2.8 |
| 9 | AI | 19 | VAL | 2.8 |
| 18 | AR | 22 | ASP | 2.8 |
| 24 | CC | 155 | ALA | 2.8 |
| 35 | DO | 9 | GLN | 2.8 |
| 40 | CT | 9 | HIS | 2.8 |
| 5 | BE | 100 | SER | 2.8 |
| 3 | BC | 201 | TRP | 2.8 |
| 14 | BN | 13 | ARG | 2.8 |
| 21 | BU | 19 | PHE | 2.8 |
| 26 | CE | 106 | LYS | 2.8 |
| 29 | CH | 68 | ARG | 2.8 |
| 35 | DO | 100 | CYS | 2.8 |
| 37 | CQ | 109 | ARG | 2.8 |
| 38 | DR | 36 | PHE | 2.8 |
| 51 | C4 | 16 | LYS | 2.8 |
| 33 | DM | 34 | GLY | 2.8 |
| 1 | BA | 145 | G | 2.8 |
| 22 | CA | 1721 | G | 2.8 |
| 23 | CB | 64 | G | 2.8 |
| 53 | DA | 570 | G | 2.8 |
| 53 | DA | 1071 | G | 2.8 |
| 1 | BA | 955 | U | 2.8 |
| 1 | BA | 1333 | A | 2.8 |
| 22 | CA | 146 | A | 2.8 |
| 22 | CA | 1586 | A | 2.8 |
| 37 | CQ | 27 | GLU | 2.8 |
| 48 | C1 | 36 | GLU | 2.8 |
| 22 | CA | 257 | C | 2.8 |
| 17 | BQ | 21 | ILE | 2.8 |
| 26 | CE | 76 | PRO | 2.8 |
| 27 | DF | 85 | ILE | 2.8 |
| 32 | CL | 99 | ILE | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 47 | C0 | 42 | PRO | 2.8 |
| 7 | AG | 118 | LEU | 2.8 |
| 7 | BG | 117 | ALA | 2.8 |
| 8 | BH | 18 | GLN | 2.8 |
| 28 | DG | 111 | HIS | 2.8 |
| 36 | CP | 77 | ALA | 2.8 |
| 38 | CR | 14 | HIS | 2.8 |
| 41 | CU | 35 | ALA | 2.8 |
| 54 | DD | 192 | ALA | 2.8 |
| 55 | DI | 3 | LEU | 2.8 |
| 6 | BF | 2 | ARG | 2.8 |
| 10 | AJ | 22 | THR | 2.8 |
| 11 | BK | 17 | SER | 2.8 |
| 19 | BS | 79 | THR | 2.8 |
| 24 | DC | 272 | SER | 2.8 |
| 35 | CO | 116 | VAL | 2.8 |
| 1 | AA | 472 | U | 2.8 |
| 8 | BH | 73 | GLU | 2.8 |
| 22 | CA | 40 | U | 2.8 |
| 38 | DR | 23 | GLY | 2.8 |
| 1 | BA | 976 | G | 2.8 |
| 1 | BA | 1036 | A | 2.8 |
| 1 | BA | 1366 | C | 2.8 |
| 10 | BJ | 13 | PHE | 2.8 |
| 22 | CA | 229 | C | 2.8 |
| 22 | CA | 2558 | C | 2.8 |
| 24 | DC | 6 | CYS | 2.8 |
| 24 | DC | 188 | CYS | 2.8 |
| 46 | CZ | 27 | ASN | 2.8 |
| 2 | AB | 122 | GLN | 2.8 |
| 19 | AS | 29 | LYS | 2.8 |
| 20 | BT | 48 | GLN | 2.8 |
| 25 | CD | 205 | PRO | 2.8 |
| 26 | CE | 185 | LYS | 2.8 |
| 27 | CF | 72 | LYS | 2.8 |
| 33 | CM | 17 | LYS | 2.8 |
| 24 | CC | 53 | HIS | 2.8 |
| 31 | DK | 77 | HIS | 2.8 |
| 42 | CV | 7 | ARG | 2.8 |
| 51 | C4 | 26 | HIS | 2.8 |
| 2 | BB | 52 | GLU | 2.8 |
| 15 | BO | 26 | GLU | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 3 | AC | 178 | LEU | 2.8 |
| 7 | BG | 22 | LEU | 2.8 |
| 8 | BH | 40 | LEU | 2.8 |
| 14 | AN | 48 | LEU | 2.8 |
| 24 | CC | 178 | SER | 2.8 |
| 26 | CE | 70 | SER | 2.8 |
| 29 | DH | 148 | ALA | 2.8 |
| 37 | CQ | 48 | ILE | 2.8 |
| 38 | CR | 9 | ILE | 2.8 |
| 39 | CS | 62 | GLU | 2.8 |
| 40 | CT | 2 | GLU | 2.8 |
| 44 | CX | 29 | GLU | 2.8 |
| 51 | C4 | 48 | ALA | 2.8 |
| 3 | BC | 90 | VAL | 2.8 |
| 19 | AS | 58 | VAL | 2.8 |
| 36 | CP | 86 | GLY | 2.8 |
| 51 | D4 | 56 | GLY | 2.8 |
| 1 | AA | 1038 | C | 2.8 |
| 22 | CA | 2794 | C | 2.8 |
| 22 | CA | 2820 | A | 2.8 |
| 23 | CB | 4 | C | 2.8 |
| 1 | AA | 846 | G | 2.8 |
| 1 | BA | 1453 | G | 2.8 |
| 22 | CA | 254 | G | 2.8 |
| 22 | CA | 953 | G | 2.8 |
| 22 | CA | 1055 | G | 2.8 |
| 22 | CA | 2307 | G | 2.8 |
| 38 | DR | 76 | TYR | 2.8 |
| 38 | CR | 22 | LYS | 2.8 |
| 45 | CY | 54 | LYS | 2.8 |
| 53 | DA | 883 | G | 2.8 |
| 33 | CM | 64 | PHE | 2.8 |
| 39 | CS | 35 | PHE | 2.8 |
| 40 | CT | 82 | MET | 2.8 |
| 1 | BA | 1211 | U | 2.8 |
| 7 | AG | 10 | ARG | 2.8 |
| 17 | AQ | 11 | ARG | 2.8 |
| 22 | CA | 102 | U | 2.8 |
| 22 | CA | 1396 | U | 2.8 |
| 35 | CO | 30 | ARG | 2.8 |
| 43 | CW | 93 | ARG | 2.8 |
| 26 | CE | 29 | HIS | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 51 | D4 | 51 | SER | 2.8 |
| 3 | BC | 160 | ALA | 2.8 |
| 24 | DC | 166 | ALA | 2.8 |
| 8 | BH | 106 | THR | 2.8 |
| 11 | AK | 92 | GLY | 2.8 |
| 16 | BP | 42 | ILE | 2.8 |
| 18 | AR | 59 | ILE | 2.8 |
| 22 | CA | 11 | C | 2.8 |
| 22 | CA | 544 | C | 2.8 |
| 22 | CA | 876 | C | 2.8 |
| 22 | CA | 1463 | C | 2.8 |
| 17 | BQ | 19 | LYS | 2.8 |
| 20 | AT | 49 | LYS | 2.8 |
| 22 | CA | 1614 | A | 2.8 |
| 22 | CA | 2317 | A | 2.8 |
| 24 | CC | 55 | GLY | 2.8 |
| 24 | CC | 135 | ILE | 2.8 |
| 24 | DC | 54 | ILE | 2.8 |
| 26 | CE | 81 | GLY | 2.8 |
| 35 | CO | 113 | ILE | 2.8 |
| 38 | DR | 65 | ILE | 2.8 |
| 51 | D4 | 57 | LEU | 2.8 |
| 25 | CD | 204 | LYS | 2.8 |
| 29 | CH | 71 | LYS | 2.8 |
| 36 | CP | 43 | ASN | 2.8 |
| 41 | DU | 92 | ASN | 2.8 |
| 1 | BA | 121 | U | 2.8 |
| 25 | CD | 164 | GLN | 2.8 |
| 7 | BG | 40 | GLU | 2.8 |
| 11 | BK | 68 | GLU | 2.8 |
| 22 | CA | 2355 | G | 2.8 |
| 22 | CA | 2375 | G | 2.8 |
| 22 | CA | 2659 | G | 2.8 |
| 35 | CO | 32 | GLU | 2.8 |
| 40 | CT | 18 | ARG | 2.8 |
| 53 | DA | 2002 | G | 2.8 |
| 53 | DA | 2618 | G | 2.8 |
| 7 | BG | 14 | PRO | 2.8 |
| 13 | BM | 91 | HIS | 2.8 |
| 16 | BP | 9 | HIS | 2.8 |
| 20 | BT | 31 | PHE | 2.8 |
| 24 | CC | 247 | PRO | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 44 | CX | 45 | PHE | 2.8 |
| 54 | DD | 134 | HIS | 2.8 |
| 26 | DE | 10 | SER | 2.8 |
| 35 | CO | 6 | SER | 2.8 |
| 55 | DI | 30 | SER | 2.8 |
| 6 | BF | 56 | LYS | 2.8 |
| 14 | BN | 3 | LYS | 2.8 |
| 26 | CE | 60 | TRP | 2.8 |
| 33 | CM | 96 | LYS | 2.8 |
| 38 | CR | 93 | LYS | 2.8 |
| 3 | BC | 93 | ASP | 2.8 |
| 5 | BE | 108 | GLY | 2.8 |
| 5 | BE | 129 | GLY | 2.8 |
| 6 | BF | 57 | ALA | 2.8 |
| 7 | AG | 127 | ALA | 2.8 |
| 19 | AS | 26 | GLY | 2.8 |
| 21 | AU | 30 | ALA | 2.8 |
| 22 | CA | 111 | A | 2.8 |
| 22 | CA | 1542 | U | 2.8 |
| 22 | CA | 2804 | U | 2.8 |
| 24 | DC | 206 | GLY | 2.8 |
| 35 | CO | 107 | ASN | 2.8 |
| 53 | DA | 2052 | A | 2.8 |
| 53 | DA | 2187 | U | 2.8 |
| 54 | DD | 115 | GLY | 2.8 |
| 54 | DD | 151 | THR | 2.8 |
| 18 | AR | 35 | GLU | 2.8 |
| 32 | DL | 110 | GLU | 2.8 |
| 9 | BI | 33 | ARG | 2.8 |
| 13 | AM | 113 | ARG | 2.8 |
| 24 | CC | 81 | LEU | 2.8 |
| 24 | CC | 156 | ARG | 2.8 |
| 32 | CL | 39 | ILE | 2.8 |
| 39 | CS | 78 | ARG | 2.8 |
| 48 | C1 | 43 | ILE | 2.8 |
| 55 | DI | 41 | LEU | 2.8 |
| 4 | BD | 25 | VAL | 2.8 |
| 25 | CD | 142 | VAL | 2.8 |
| 2 | BB | 143 | LYS | 2.7 |
| 22 | CA | 321 | U | 2.7 |
| 31 | CK | 74 | TYR | 2.7 |
| 4 | AD | 138 | SER | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 17 | BQ | 72 | SER | 2.7 |
| 23 | CB | 60 | C | 2.7 |
| 2 | AB | 127 | ASP | 2.7 |
| 33 | DM | 50 | PHE | 2.7 |
| 34 | CN | 68 | PHE | 2.7 |
| 35 | DO | 21 | PHE | 2.7 |
| 3 | BC | 21 | THR | 2.7 |
| 19 | AS | 32 | ARG | 2.7 |
| 35 | CO | 104 | ALA | 2.7 |
| 36 | CP | 23 | ALA | 2.7 |
| 37 | CQ | 93 | ARG | 2.7 |
| 38 | CR | 12 | ALA | 2.7 |
| 3 | BC | 43 | LEU | 2.7 |
| 13 | AM | 89 | LEU | 2.7 |
| 14 | AN | 82 | ILE | 2.7 |
| 34 | CN | 78 | LEU | 2.7 |
| 39 | CS | 24 | LYS | 2.7 |
| 41 | CU | 19 | LYS | 2.7 |
| 3 | BC | 66 | VAL | 2.7 |
| 5 | AE | 56 | VAL | 2.7 |
| 8 | AH | 25 | VAL | 2.7 |
| 22 | CA | 43 | G | 2.7 |
| 22 | CA | 1455 | G | 2.7 |
| 23 | CB | 10 | G | 2.7 |
| 34 | CN | 26 | VAL | 2.7 |
| 34 | CN | 93 | VAL | 2.7 |
| 37 | DQ | 46 | VAL | 2.7 |
| 3 | BC | 3 | GLN | 2.7 |
| 14 | BN | 5 | SER | 2.7 |
| 20 | BT | 6 | SER | 2.7 |
| 22 | CA | 364 | C | 2.7 |
| 32 | CL | 106 | GLU | 2.7 |
| 33 | CM | 136 | GLU | 2.7 |
| 39 | CS | 31 | GLU | 2.7 |
| 31 | CK | 49 | ASP | 2.7 |
| 35 | DO | 119 | SER | 2.7 |
| 53 | DA | 1868 | C | 2.7 |
| 3 | AC | 2 | GLY | 2.7 |
| 5 | BE | 50 | TYR | 2.7 |
| 8 | BH | 65 | TYR | 2.7 |
| 9 | AI | 45 | ARG | 2.7 |
| 22 | CA | 1858 | A | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 32 | CL | 49 | ARG | 2.7 |
| 33 | CM | 47 | ARG | 2.7 |
| 48 | C1 | 17 | ARG | 2.7 |
| 11 | AK | 73 | ALA | 2.7 |
| 24 | CC | 173 | THR | 2.7 |
| 33 | CM | 9 | ALA | 2.7 |
| 38 | DR | 21 | ALA | 2.7 |
| 54 | DD | 171 | THR | 2.7 |
| 14 | BN | 6 | MET | 2.7 |
| 16 | BP | 15 | PRO | 2.7 |
| 22 | CA | 1862 | G | 2.7 |
| 22 | CA | 2341 | G | 2.7 |
| 24 | CC | 164 | ILE | 2.7 |
| 25 | CD | 2 | ILE | 2.7 |
| 26 | CE | 30 | GLN | 2.7 |
| 26 | CE | 78 | TRP | 2.7 |
| 29 | DH | 94 | ILE | 2.7 |
| 38 | CR | 60 | LEU | 2.7 |
| 51 | C4 | 55 | LEU | 2.7 |
| 52 | C5 | 23 | ILE | 2.7 |
| 2 | AB | 210 | VAL | 2.7 |
| 24 | CC | 4 | VAL | 2.7 |
| 25 | CD | 178 | VAL | 2.7 |
| 26 | CE | 49 | ARG | 2.7 |
| 38 | CR | 53 | ARG | 2.7 |
| 42 | CV | 93 | VAL | 2.7 |
| 51 | C4 | 8 | ARG | 2.7 |
| 22 | CA | 1204 | A | 2.7 |
| 1 | BA | 1451 | U | 2.7 |
| 22 | CA | 667 | U | 2.7 |
| 32 | CL | 15 | GLY | 2.7 |
| 51 | C4 | 9 | GLY | 2.7 |
| 12 | BL | 18 | LYS | 2.7 |
| 14 | BN | 98 | LYS | 2.7 |
| 26 | CE | 132 | LYS | 2.7 |
| 2 | BB | 90 | PHE | 2.7 |
| 24 | CC | 51 | THR | 2.7 |
| 28 | CG | 7 | ALA | 2.7 |
| 1 | AA | 1137 | C | 2.7 |
| 1 | BA | 1228 | C | 2.7 |
| 1 | BA | 1237 | C | 2.7 |
| 1 | BA | 1262 | C | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 18 | BR | 74 | HIS | 2.7 |
| 13 | AM | 11 | ASP | 2.7 |
| 28 | DG | 166 | ASP | 2.7 |
| 1 | BA | 1323 | G | 2.7 |
| 5 | AE | 70 | ASN | 2.7 |
| 13 | BM | 112 | PRO | 2.7 |
| 21 | BU | 21 | ARG | 2.7 |
| 24 | CC | 101 | ARG | 2.7 |
| 34 | CN | 40 | ARG | 2.7 |
| 1 | BA | 1346 | A | 2.7 |
| 5 | BE | 115 | LEU | 2.7 |
| 22 | CA | 1223 | G | 2.7 |
| 53 | DA | 1174 | U | 2.7 |
| 54 | DD | 165 | MET | 2.7 |
| 8 | AH | 50 | LYS | 2.7 |
| 9 | AI | 68 | LYS | 2.7 |
| 22 | CA | 941 | A | 2.7 |
| 45 | CY | 2 | SER | 2.7 |
| 47 | C0 | 12 | SER | 2.7 |
| 30 | DJ | 109 | ILE | 2.7 |
| 39 | CS | 73 | LYS | 2.7 |
| 46 | CZ | 2 | LYS | 2.7 |
| 51 | C4 | 41 | LYS | 2.7 |
| 3 | AC | 128 | VAL | 2.7 |
| 3 | BC | 18 | TRP | 2.7 |
| 17 | AQ | 46 | VAL | 2.7 |
| 24 | CC | 216 | VAL | 2.7 |
| 24 | DC | 56 | GLY | 2.7 |
| 31 | DK | 48 | VAL | 2.7 |
| 25 | CD | 17 | GLU | 2.7 |
| 2 | AB | 211 | THR | 2.7 |
| 6 | BF | 77 | THR | 2.7 |
| 7 | AG | 44 | TYR | 2.7 |
| 48 | D1 | 5 | GLN | 2.7 |
| 1 | AA | 1001 | C | 2.7 |
| 15 | BO | 74 | ASP | 2.7 |
| 22 | CA | 931 | U | 2.7 |
| 23 | CB | 113 | C | 2.7 |
| 24 | CC | 238 | ARG | 2.7 |
| 26 | CE | 176 | ASP | 2.7 |
| 31 | CK | 4 | PHE | 2.7 |
| 34 | CN | 31 | PHE | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 50 | C3 | 41 | ARG | 2.7 |
| 14 | BN | 76 | LYS | 2.7 |
| 29 | CH | 119 | ASN | 2.7 |
| 35 | CO | 23 | ASN | 2.7 |
| 19 | BS | 9 | PRO | 2.7 |
| 13 | BM | 49 | SER | 2.7 |
| 22 | CA | 1373 | A | 2.7 |
| 23 | CB | 15 | A | 2.7 |
| 3 | BC | 82 | GLU | 2.7 |
| 22 | CA | 1527 | G | 2.7 |
| 22 | CA | 2162 | G | 2.7 |
| 23 | CB | 24 | G | 2.7 |
| 53 | DA | 1660 | G | 2.7 |
| 53 | DA | 2053 | G | 2.7 |
| 54 | DD | 139 | SER | 2.7 |
| 24 | CC | 42 | GLY | 2.7 |
| 42 | CV | 90 | GLY | 2.7 |
| 20 | BT | 39 | ILE | 2.7 |
| 44 | DX | 37 | ILE | 2.7 |
| 1 | AA | 1168 | U | 2.7 |
| 26 | CE | 195 | GLN | 2.7 |
| 38 | CR | 88 | VAL | 2.7 |
| 54 | DD | 148 | GLN | 2.7 |
| 1 | BA | 1234 | C | 2.7 |
| 2 | AB | 113 | ARG | 2.7 |
| 2 | AB | 192 | ASP | 2.7 |
| 22 | CA | 2651 | C | 2.7 |
| 24 | CC | 52 | ARG | 2.7 |
| 26 | CE | 162 | ARG | 2.7 |
| 36 | CP | 89 | ASP | 2.7 |
| 38 | CR | 102 | ASP | 2.7 |
| 3 | BC | 113 | ALA | 2.7 |
| 7 | AG | 84 | THR | 2.7 |
| 10 | AJ | 21 | ALA | 2.7 |
| 19 | AS | 6 | LYS | 2.7 |
| 21 | AU | 43 | THR | 2.7 |
| 24 | DC | 191 | THR | 2.7 |
| 32 | CL | 114 | LYS | 2.7 |
| 36 | CP | 24 | THR | 2.7 |
| 40 | CT | 89 | ALA | 2.7 |
| 45 | CY | 14 | THR | 2.7 |
| 2 | AB | 145 | GLU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 13 | BM | 66 | GLU | 2.7 |
| 1 | BA | 181 | A | 2.7 |
| 22 | CA | 152 | A | 2.7 |
| 27 | DF | 114 | PHE | 2.7 |
| 35 | CO | 87 | PHE | 2.7 |
| 30 | DJ | 117 | MET | 2.7 |
| 22 | CA | 974 | G | 2.7 |
| 22 | CA | 1031 | G | 2.7 |
| 22 | CA | 2002 | G | 2.7 |
| 23 | CB | 18 | G | 2.7 |
| 38 | DR | 7 | GLY | 2.7 |
| 47 | C0 | 15 | GLY | 2.7 |
| 53 | DA | 895 | U | 2.7 |
| 53 | DA | 2188 | U | 2.7 |
| 54 | DD | 158 | GLY | 2.7 |
| 8 | BH | 99 | LEU | 2.6 |
| 6 | BF | 44 | ARG | 2.6 |
| 3 | BC | 10 | ILE | 2.6 |
| 7 | BG | 12 | ILE | 2.6 |
| 32 | DL | 77 | ILE | 2.6 |
| 39 | CS | 85 | LYS | 2.6 |
| 4 | AD | 25 | VAL | 2.6 |
| 7 | AG | 75 | VAL | 2.6 |
| 25 | CD | 37 | VAL | 2.6 |
| 37 | CQ | 81 | VAL | 2.6 |
| 25 | CD | 58 | ASN | 2.6 |
| 36 | CP | 31 | THR | 2.6 |
| 38 | DR | 42 | ALA | 2.6 |
| 39 | CS | 28 | ALA | 2.6 |
| 22 | CA | 482 | A | 2.6 |
| 10 | AJ | 39 | PRO | 2.6 |
| 22 | CA | 1457 | U | 2.6 |
| 53 | DA | 1821 | A | 2.6 |
| 19 | BS | 35 | SER | 2.6 |
| 31 | DK | 75 | TYR | 2.6 |
| 33 | DM | 58 | TYR | 2.6 |
| 51 | D4 | 64 | TYR | 2.6 |
| 11 | BK | 19 | GLY | 2.6 |
| 31 | CK | 89 | PHE | 2.6 |
| 33 | CM | 45 | GLY | 2.6 |
| 33 | CM | 88 | GLY | 2.6 |
| 39 | CS | 77 | PHE | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 46 | DZ | 62 | GLY | 2.6 |
| 2 | AB | 64 | LYS | 2.6 |
| 22 | CA | 48 | G | 2.6 |
| 22 | CA | 1149 | G | 2.6 |
| 22 | CA | 2405 | G | 2.6 |
| 7 | AG | 143 | ARG | 2.6 |
| 40 | CT | 84 | ARG | 2.6 |
| 45 | CY | 3 | ARG | 2.6 |
| 48 | C1 | 7 | LYS | 2.6 |
| 49 | D2 | 30 | LYS | 2.6 |
| 1 | BA | 1273 | C | 2.6 |
| 22 | CA | 1816 | C | 2.6 |
| 37 | CQ | 11 | GLU | 2.6 |
| 24 | DC | 105 | LEU | 2.6 |
| 31 | CK | 32 | LEU | 2.6 |
| 37 | CQ | 115 | ASN | 2.6 |
| 51 | D4 | 55 | LEU | 2.6 |
| 5 | BE | 60 | ILE | 2.6 |
| 1 | BA | 1035 | A | 2.6 |
| 24 | DC | 228 | VAL | 2.6 |
| 41 | CU | 86 | THR | 2.6 |
| 55 | DI | 54 | VAL | 2.6 |
| 45 | CY | 69 | ALA | 2.6 |
| 46 | CZ | 51 | ALA | 2.6 |
| 55 | DI | 80 | THR | 2.6 |
| 2 | BB | 48 | PRO | 2.6 |
| 26 | CE | 110 | SER | 2.6 |
| 37 | CQ | 65 | SER | 2.6 |
| 48 | D1 | 11 | SER | 2.6 |
| 55 | DI | 24 | SER | 2.6 |
| 40 | CT | 27 | LYS | 2.6 |
| 21 | BU | 17 | ARG | 2.6 |
| 26 | CE | 71 | GLY | 2.6 |
| 24 | CC | 248 | TRP | 2.6 |
| 25 | CD | 141 | ARG | 2.6 |
| 31 | DK | 79 | GLY | 2.6 |
| 54 | DD | 166 | GLY | 2.6 |
| 22 | CA | 1016 | G | 2.6 |
| 22 | CA | 1600 | C | 2.6 |
| 32 | CL | 37 | ASP | 2.6 |
| 22 | CA | 2825 | G | 2.6 |
| 23 | CB | 41 | G | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-------|------|------|
| 53 | DA | 2024 | G | 2.6 |
| 24 | CC | 45 | ASN | 2.6 |
| 33 | CM | 6 | LEU | 2.6 |
| 33 | DM | 57 | LEU | 2.6 |
| 53 | DA | 2823 | A | 2.6 |
| 26 | CE | 47 | LYS | 2.6 |
| 35 | CO | 18 | GLN | 2.6 |
| 40 | CT | 6 | LYS | 2.6 |
| 46 | DZ | 4 | LYS | 2.6 |
| 9 | BI | 28 | ILE | 2.6 |
| 21 | BU | 42 | THR | 2.6 |
| 36 | CP | 8 | ILE | 2.6 |
| 37 | DQ | 36 | SER | 2.6 |
| 54 | DD | 133 | THR | 2.6 |
| 11 | AK | 56 | ARG | 2.6 |
| 16 | AP | 27 | ALA | 2.6 |
| 24 | CC | 76 | ALA | 2.6 |
| 24 | DC | 156 | ARG | 2.6 |
| 25 | CD | 209 | ALA | 2.6 |
| 26 | CE | 161 | ALA | 2.6 |
| 31 | CK | 73 | VAL | 2.6 |
| 40 | CT | 20 | VAL | 2.6 |
| 40 | CT | 47 | VAL | 2.6 |
| 44 | DX | 41[A] | ARG | 2.6 |
| 2 | AB | 180 | GLY | 2.6 |
| 3 | BC | 9 | GLY | 2.6 |
| 9 | AI | 8 | GLY | 2.6 |
| 12 | BL | 92 | GLY | 2.6 |
| 22 | CA | 76 | C | 2.6 |
| 22 | CA | 292 | U | 2.6 |
| 22 | CA | 341 | C | 2.6 |
| 22 | CA | 2798 | U | 2.6 |
| 24 | DC | 12 | GLY | 2.6 |
| 30 | DJ | 32 | GLY | 2.6 |
| 44 | DX | 22 | GLY | 2.6 |
| 54 | DD | 163 | GLY | 2.6 |
| 12 | BL | 46 | ASN | 2.6 |
| 22 | CA | 7 | G | 2.6 |
| 22 | CA | 51 | G | 2.6 |
| 22 | CA | 1389 | G | 2.6 |
| 53 | DA | 1661 | G | 2.6 |
| 53 | DA | 2141 | G | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 6 | BF | 42 | TRP | 2.6 |
| 21 | BU | 23 | CYS | 2.6 |
| 24 | CC | 188 | CYS | 2.6 |
| 37 | CQ | 31 | TRP | 2.6 |
| 49 | C2 | 19 | HIS | 2.6 |
| 2 | AB | 59 | LYS | 2.6 |
| 3 | AC | 86 | LYS | 2.6 |
| 14 | AN | 28 | LYS | 2.6 |
| 49 | C2 | 39 | PHE | 2.6 |
| 22 | CA | 2134 | A | 2.6 |
| 53 | DA | 2614 | A | 2.6 |
| 16 | BP | 74 | LEU | 2.6 |
| 36 | CP | 13 | ARG | 2.6 |
| 39 | CS | 79 | ARG | 2.6 |
| 46 | CZ | 52 | ARG | 2.6 |
| 53 | DA | 137 | U | 2.6 |
| 7 | AG | 16 | PRO | 2.6 |
| 7 | AG | 133 | THR | 2.6 |
| 11 | AK | 72 | ASP | 2.6 |
| 40 | CT | 72 | THR | 2.6 |
| 1 | AA | 206 | C | 2.6 |
| 1 | BA | 215 | C | 2.6 |
| 1 | BA | 1320 | C | 2.6 |
| 1 | BA | 1322 | C | 2.6 |
| 2 | AB | 61 | ALA | 2.6 |
| 4 | AD | 24 | GLY | 2.6 |
| 22 | CA | 723 | C | 2.6 |
| 23 | CB | 28 | C | 2.6 |
| 17 | BQ | 38 | ILE | 2.6 |
| 24 | CC | 99 | GLY | 2.6 |
| 26 | CE | 39 | ALA | 2.6 |
| 29 | DH | 23 | ALA | 2.6 |
| 38 | DR | 38 | ALA | 2.6 |
| 39 | DS | 74 | ILE | 2.6 |
| 51 | C4 | 27 | ALA | 2.6 |
| 16 | BP | 36 | VAL | 2.6 |
| 40 | DT | 50 | VAL | 2.6 |
| 54 | DD | 170 | VAL | 2.6 |
| 22 | CA | 81 | G | 2.6 |
| 22 | CA | 215 | G | 2.6 |
| 32 | CL | 67 | LYS | 2.6 |
| 35 | CO | 42 | LYS | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 44 | CX | 72 | LYS | 2.6 |
| 47 | C0 | 34 | HIS | 2.6 |
| 25 | CD | 88 | GLU | 2.6 |
| 55 | DI | 6 | GLN | 2.6 |
| 14 | BN | 85 | ARG | 2.6 |
| 22 | CA | 90 | U | 2.6 |
| 22 | CA | 103 | A | 2.6 |
| 22 | CA | 355 | U | 2.6 |
| 22 | CA | 2377 | A | 2.6 |
| 24 | CC | 177 | ARG | 2.6 |
| 35 | CO | 4 | ARG | 2.6 |
| 38 | DR | 47 | TYR | 2.6 |
| 4 | AD | 182 | PHE | 2.6 |
| 11 | AK | 61 | PHE | 2.6 |
| 26 | DE | 85 | PHE | 2.6 |
| 50 | D3 | 5 | PHE | 2.6 |
| 55 | DI | 69 | PHE | 2.6 |
| 9 | AI | 62 | ASP | 2.6 |
| 34 | CN | 92 | TRP | 2.6 |
| 19 | AS | 25 | SER | 2.6 |
| 22 | CA | 440 | C | 2.6 |
| 40 | CT | 81 | SER | 2.6 |
| 53 | DA | 2000 | C | 2.6 |
| 2 | AB | 125 | THR | 2.6 |
| 3 | BC | 109 | PRO | 2.6 |
| 5 | BE | 44 | GLY | 2.6 |
| 8 | BH | 92 | LEU | 2.6 |
| 12 | BL | 7 | LEU | 2.6 |
| 35 | CO | 65 | LEU | 2.6 |
| 35 | DO | 44 | LEU | 2.6 |
| 48 | D1 | 14 | GLY | 2.6 |
| 2 | AB | 76 | ALA | 2.6 |
| 35 | CO | 108 | ALA | 2.6 |
| 35 | DO | 108 | ALA | 2.6 |
| 37 | CQ | 29 | LYS | 2.6 |
| 51 | D4 | 10 | ALA | 2.6 |
| 1 | BA | 1301 | U | 2.6 |
| 3 | AC | 66 | VAL | 2.6 |
| 18 | AR | 21 | ILE | 2.6 |
| 24 | DC | 201 | MET | 2.6 |
| 25 | CD | 165 | MET | 2.6 |
| 16 | BP | 18 | GLN | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 17 | AQ | 78 | VAL | 2.6 |
| 22 | CA | 2302 | U | 2.6 |
| 24 | CC | 17 | VAL | 2.6 |
| 25 | CD | 172 | VAL | 2.6 |
| 49 | C2 | 9 | ILE | 2.6 |
| 17 | BQ | 47 | HIS | 2.6 |
| 1 | BA | 1048 | G | 2.6 |
| 1 | BA | 1290 | G | 2.6 |
| 2 | BB | 21 | ARG | 2.6 |
| 7 | BG | 95 | ARG | 2.6 |
| 23 | CB | 6 | G | 2.6 |
| 1 | BA | 946 | A | 2.6 |
| 1 | BA | 1446 | A | 2.6 |
| 22 | CA | 255 | A | 2.6 |
| 22 | CA | 497 | A | 2.6 |
| 16 | BP | 53 | ASP | 2.6 |
| 27 | DF | 147 | ASP | 2.6 |
| 1 | AA | 73 | C | 2.6 |
| 1 | AA | 841 | C | 2.6 |
| 22 | CA | 1049 | C | 2.6 |
| 22 | CA | 1592 | C | 2.6 |
| 53 | DA | 2001 | C | 2.6 |
| 2 | BB | 50 | PHE | 2.5 |
| 3 | AC | 187 | SER | 2.5 |
| 21 | AU | 37 | PHE | 2.5 |
| 24 | CC | 11 | PRO | 2.5 |
| 25 | CD | 152 | PRO | 2.5 |
| 27 | CF | 139 | PRO | 2.5 |
| 52 | C5 | 32 | LYS | 2.5 |
| 1 | AA | 92 | U | 2.5 |
| 9 | AI | 92 | GLU | 2.5 |
| 24 | CC | 241 | GLY | 2.5 |
| 25 | CD | 28 | GLU | 2.5 |
| 48 | C1 | 14 | GLY | 2.5 |
| 51 | D4 | 53 | GLY | 2.5 |
| 8 | BH | 21 | ASN | 2.5 |
| 11 | BK | 121 | CYS | 2.5 |
| 12 | BL | 58 | THR | 2.5 |
| 24 | CC | 134 | ASN | 2.5 |
| 26 | CE | 53 | THR | 2.5 |
| 31 | DK | 78 | THR | 2.5 |
| 35 | DO | 11 | ASN | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 5 | BE | 36 | LEU | 2.5 |
| 5 | BE | 110 | ALA | 2.5 |
| 9 | AI | 87 | LEU | 2.5 |
| 25 | CD | 4 | LEU | 2.5 |
| 38 | CR | 118 | ALA | 2.5 |
| 5 | BE | 54 | ARG | 2.5 |
| 11 | AK | 37 | ARG | 2.5 |
| 21 | AU | 45 | ARG | 2.5 |
| 38 | CR | 6 | ARG | 2.5 |
| 1 | AA | 1453 | G | 2.5 |
| 2 | BB | 163 | VAL | 2.5 |
| 4 | BD | 132 | ILE | 2.5 |
| 5 | BE | 123 | VAL | 2.5 |
| 6 | BF | 64 | VAL | 2.5 |
| 14 | AN | 84 | VAL | 2.5 |
| 17 | AQ | 13 | VAL | 2.5 |
| 22 | CA | 173 | A | 2.5 |
| 22 | CA | 347 | A | 2.5 |
| 22 | CA | 1548 | A | 2.5 |
| 22 | CA | 1654 | A | 2.5 |
| 25 | CD | 189 | VAL | 2.5 |
| 25 | CD | 203 | VAL | 2.5 |
| 32 | CL | 24 | VAL | 2.5 |
| 38 | DR | 62 | ILE | 2.5 |
| 47 | C0 | 40 | ASP | 2.5 |
| 53 | DA | 2018 | G | 2.5 |
| 11 | BK | 14 | LYS | 2.5 |
| 20 | BT | 71 | LYS | 2.5 |
| 22 | CA | 66 | C | 2.5 |
| 22 | CA | 517 | C | 2.5 |
| 22 | CA | 2213 | U | 2.5 |
| 42 | CV | 10 | GLU | 2.5 |
| 2 | AB | 51 | ASN | 2.5 |
| 2 | BB | 36 | ASN | 2.5 |
| 24 | DC | 218 | PRO | 2.5 |
| 33 | DM | 65 | GLY | 2.5 |
| 35 | CO | 93 | GLY | 2.5 |
| 40 | DT | 87 | PRO | 2.5 |
| 51 | C4 | 63 | PRO | 2.5 |
| 32 | CL | 31 | ARG | 2.5 |
| 36 | CP | 15 | ARG | 2.5 |
| 3 | BC | 48 | ALA | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 9 | BI | 78 | ALA | 2.5 |
| 24 | DC | 208 | ALA | 2.5 |
| 43 | CW | 80 | HIS | 2.5 |
| 22 | CA | 91 | A | 2.5 |
| 22 | CA | 219 | A | 2.5 |
| 22 | CA | 1096 | A | 2.5 |
| 22 | CA | 2800 | A | 2.5 |
| 45 | CY | 5 | CYS | 2.5 |
| 1 | BA | 1168 | U | 2.5 |
| 2 | BB | 115 | LYS | 2.5 |
| 16 | BP | 12 | LYS | 2.5 |
| 19 | BS | 34 | TRP | 2.5 |
| 1 | BA | 1249 | C | 2.5 |
| 22 | CA | 295 | G | 2.5 |
| 22 | CA | 1355 | G | 2.5 |
| 22 | CA | 1547 | C | 2.5 |
| 22 | CA | 1568 | G | 2.5 |
| 22 | CA | 2313 | C | 2.5 |
| 53 | DA | 2122 | U | 2.5 |
| 53 | DA | 1867 | G | 2.5 |
| 3 | AC | 91 | VAL | 2.5 |
| 5 | AE | 60 | ILE | 2.5 |
| 5 | BE | 72 | ILE | 2.5 |
| 11 | BK | 129 | VAL | 2.5 |
| 20 | BT | 35 | VAL | 2.5 |
| 25 | CD | 107 | VAL | 2.5 |
| 35 | DO | 47 | VAL | 2.5 |
| 40 | CT | 55 | ILE | 2.5 |
| 44 | DX | 23 | VAL | 2.5 |
| 3 | BC | 154 | SER | 2.5 |
| 9 | BI | 96 | SER | 2.5 |
| 5 | AE | 79 | GLY | 2.5 |
| 25 | CD | 126 | ASN | 2.5 |
| 11 | AK | 98 | ARG | 2.5 |
| 33 | DM | 31 | GLY | 2.5 |
| 48 | D1 | 10 | ARG | 2.5 |
| 49 | C2 | 41 | PRO | 2.5 |
| 51 | C4 | 53 | GLY | 2.5 |
| 5 | AE | 24 | THR | 2.5 |
| 9 | BI | 60 | LYS | 2.5 |
| 9 | BI | 115 | LYS | 2.5 |
| 14 | AN | 38 | ASP | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 24 | CC | 18 | LYS | 2.5 |
| 39 | CS | 82 | HIS | 2.5 |
| 38 | CR | 57 | PHE | 2.5 |
| 44 | CX | 24 | LYS | 2.5 |
| 2 | AB | 223 | GLU | 2.5 |
| 7 | BG | 21 | GLU | 2.5 |
| 22 | CA | 233 | A | 2.5 |
| 22 | CA | 1205 | A | 2.5 |
| 24 | CC | 166 | ALA | 2.5 |
| 34 | DN | 82 | MET | 2.5 |
| 51 | D4 | 14 | PHE | 2.5 |
| 34 | CN | 124 | LEU | 2.5 |
| 1 | BA | 633 | G | 2.5 |
| 22 | CA | 1358 | G | 2.5 |
| 22 | CA | 1410 | G | 2.5 |
| 22 | CA | 1715 | G | 2.5 |
| 22 | CA | 2116 | G | 2.5 |
| 53 | DA | 2363 | G | 2.5 |
| 2 | AB | 222 | ARG | 2.5 |
| 6 | AF | 103 | VAL | 2.5 |
| 14 | AN | 55 | SER | 2.5 |
| 16 | AP | 79 | ASN | 2.5 |
| 16 | BP | 25 | ARG | 2.5 |
| 28 | DG | 10 | VAL | 2.5 |
| 29 | DH | 20 | ASN | 2.5 |
| 29 | DH | 110 | VAL | 2.5 |
| 34 | CN | 6 | ARG | 2.5 |
| 39 | CS | 58 | VAL | 2.5 |
| 50 | C3 | 38 | GLY | 2.5 |
| 2 | AB | 48 | PRO | 2.5 |
| 48 | D1 | 7 | LYS | 2.5 |
| 5 | BE | 145 | GLU | 2.5 |
| 49 | C2 | 51 | GLU | 2.5 |
| 11 | BK | 18 | ASP | 2.5 |
| 24 | CC | 230 | HIS | 2.5 |
| 26 | DE | 7 | ASP | 2.5 |
| 1 | BA | 959 | A | 2.5 |
| 24 | CC | 50 | THR | 2.5 |
| 26 | DE | 84 | THR | 2.5 |
| 31 | CK | 78 | THR | 2.5 |
| 1 | BA | 980 | C | 2.5 |
| 22 | CA | 420 | C | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 53 | DA | 1652 | A | 2.5 |
| 53 | DA | 2577 | A | 2.5 |
| 5 | AE | 99 | ALA | 2.5 |
| 6 | BF | 27 | ALA | 2.5 |
| 26 | DE | 87 | ALA | 2.5 |
| 27 | DF | 43 | ALA | 2.5 |
| 32 | CL | 7 | MET | 2.5 |
| 34 | CN | 82 | MET | 2.5 |
| 38 | CR | 32 | TYR | 2.5 |
| 42 | CV | 64 | ALA | 2.5 |
| 42 | DV | 51 | ALA | 2.5 |
| 16 | BP | 32 | PHE | 2.5 |
| 19 | AS | 56 | GLN | 2.5 |
| 1 | BA | 947 | G | 2.5 |
| 2 | BB | 93 | ASN | 2.5 |
| 7 | AG | 66 | LEU | 2.5 |
| 14 | BN | 90 | ARG | 2.5 |
| 22 | CA | 85 | G | 2.5 |
| 22 | CA | 333 | G | 2.5 |
| 22 | CA | 1421 | G | 2.5 |
| 22 | CA | 2838 | G | 2.5 |
| 23 | CB | 44 | G | 2.5 |
| 53 | DA | 2148 | G | 2.5 |
| 54 | DD | 167 | ASN | 2.5 |
| 9 | BI | 100 | LYS | 2.5 |
| 10 | BJ | 82 | LYS | 2.5 |
| 34 | CN | 107 | GLY | 2.5 |
| 34 | CN | 133 | LYS | 2.5 |
| 35 | DO | 15 | SER | 2.5 |
| 40 | CT | 83 | LYS | 2.5 |
| 20 | AT | 40 | GLU | 2.5 |
| 29 | CH | 76 | GLU | 2.5 |
| 45 | DY | 15 | GLY | 2.5 |
| 50 | C3 | 17 | GLY | 2.5 |
| 2 | AB | 70 | VAL | 2.5 |
| 2 | BB | 173 | ILE | 2.5 |
| 3 | BC | 173 | VAL | 2.5 |
| 3 | BC | 195 | VAL | 2.5 |
| 9 | AI | 111 | VAL | 2.5 |
| 10 | BJ | 63 | ASP | 2.5 |
| 25 | CD | 39 | ASP | 2.5 |
| 25 | CD | 80 | TRP | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 40 | DT | 103 | ILE | 2.5 |
| 52 | D5 | 26 | ILE | 2.5 |
| 1 | BA | 1318 | A | 2.5 |
| 22 | CA | 515 | A | 2.5 |
| 50 | C3 | 4 | THR | 2.5 |
| 2 | AB | 89 | GLN | 2.5 |
| 10 | AJ | 20 | GLN | 2.5 |
| 11 | AK | 38 | GLN | 2.5 |
| 19 | AS | 75 | ALA | 2.5 |
| 27 | DF | 178 | ARG | 2.5 |
| 35 | DO | 19 | ALA | 2.5 |
| 21 | BU | 54 | LYS | 2.5 |
| 31 | CK | 23 | LYS | 2.5 |
| 31 | CK | 61 | LYS | 2.5 |
| 31 | CK | 44 | TYR | 2.5 |
| 3 | AC | 47 | LEU | 2.5 |
| 12 | BL | 90 | LEU | 2.5 |
| 22 | CA | 583 | G | 2.5 |
| 22 | CA | 1423 | G | 2.5 |
| 22 | CA | 1823 | G | 2.5 |
| 24 | CC | 235 | GLY | 2.5 |
| 24 | DC | 235 | GLY | 2.5 |
| 34 | CN | 29 | GLY | 2.5 |
| 45 | CY | 33 | LEU | 2.5 |
| 7 | BG | 113 | ASP | 2.5 |
| 1 | AA | 1017 | U | 2.5 |
| 1 | BA | 468 | A | 2.5 |
| 1 | BA | 1014 | A | 2.5 |
| 1 | BA | 1239 | A | 2.5 |
| 6 | BF | 3 | HIS | 2.5 |
| 22 | CA | 443 | A | 2.5 |
| 22 | CA | 845 | A | 2.5 |
| 22 | CA | 1585 | C | 2.5 |
| 23 | CB | 110 | C | 2.5 |
| 2 | AB | 196 | VAL | 2.5 |
| 3 | AC | 14 | ILE | 2.5 |
| 5 | AE | 88 | VAL | 2.5 |
| 25 | CD | 193 | VAL | 2.5 |
| 43 | CW | 65 | VAL | 2.5 |
| 44 | CX | 51 | VAL | 2.5 |
| 3 | BC | 89 | LYS | 2.5 |
| 31 | CK | 69 | ARG | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-------|------|------|
| 34 | DN | 18[A] | ARG | 2.5 |
| 38 | CR | 51 | ARG | 2.5 |
| 50 | C3 | 19 | ARG | 2.5 |
| 35 | CO | 13 | ASN | 2.4 |
| 2 | AB | 121 | SER | 2.4 |
| 15 | BO | 13 | SER | 2.4 |
| 49 | C2 | 14 | SER | 2.4 |
| 1 | AA | 1138 | G | 2.4 |
| 1 | BA | 257 | G | 2.4 |
| 1 | BA | 950 | U | 2.4 |
| 3 | AC | 37 | PHE | 2.4 |
| 16 | BP | 17 | TYR | 2.4 |
| 22 | CA | 214 | G | 2.4 |
| 25 | CD | 3 | GLY | 2.4 |
| 33 | CM | 58 | TYR | 2.4 |
| 35 | DO | 26 | GLY | 2.4 |
| 22 | CA | 1725 | U | 2.4 |
| 1 | AA | 469 | C | 2.4 |
| 22 | CA | 2310 | C | 2.4 |
| 31 | CK | 113 | PRO | 2.4 |
| 51 | D4 | 2 | PRO | 2.4 |
| 1 | BA | 1285 | A | 2.4 |
| 1 | BA | 1339 | A | 2.4 |
| 22 | CA | 1553 | A | 2.4 |
| 14 | AN | 12 | LYS | 2.4 |
| 20 | AT | 53 | GLU | 2.4 |
| 25 | CD | 116 | LYS | 2.4 |
| 29 | CH | 50 | ARG | 2.4 |
| 29 | CH | 87 | GLU | 2.4 |
| 38 | CR | 3 | ARG | 2.4 |
| 12 | BL | 79 | VAL | 2.4 |
| 27 | DF | 74 | VAL | 2.4 |
| 45 | CY | 51 | VAL | 2.4 |
| 31 | DK | 108 | MET | 2.4 |
| 16 | BP | 7 | ALA | 2.4 |
| 18 | BR | 27 | ALA | 2.4 |
| 24 | CC | 89 | ALA | 2.4 |
| 28 | DG | 13 | ALA | 2.4 |
| 3 | BC | 187 | SER | 2.4 |
| 24 | CC | 88 | SER | 2.4 |
| 33 | CM | 34 | GLY | 2.4 |
| 33 | CM | 139 | GLY | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | CA | 1461 | C | 2.4 |
| 1 | BA | 1454 | G | 2.4 |
| 1 | BA | 466 | A | 2.4 |
| 10 | AJ | 4 | GLN | 2.4 |
| 22 | CA | 1110 | G | 2.4 |
| 22 | CA | 1311 | G | 2.4 |
| 22 | CA | 2731 | G | 2.4 |
| 53 | DA | 690 | G | 2.4 |
| 53 | DA | 1659 | G | 2.4 |
| 9 | BI | 99 | ARG | 2.4 |
| 22 | CA | 2792 | A | 2.4 |
| 24 | CC | 63 | ARG | 2.4 |
| 35 | CO | 3 | HIS | 2.4 |
| 38 | CR | 24 | TYR | 2.4 |
| 29 | CH | 30 | LEU | 2.4 |
| 38 | CR | 36 | PHE | 2.4 |
| 51 | D4 | 22 | PHE | 2.4 |
| 1 | AA | 1286 | U | 2.4 |
| 22 | CA | 416 | U | 2.4 |
| 8 | BH | 34 | VAL | 2.4 |
| 10 | AJ | 88 | MET | 2.4 |
| 24 | DC | 263 | THR | 2.4 |
| 25 | CD | 43 | ASP | 2.4 |
| 26 | DE | 43 | THR | 2.4 |
| 35 | CO | 1 | MET | 2.4 |
| 48 | C1 | 9 | THR | 2.4 |
| 54 | DD | 129 | THR | 2.4 |
| 17 | AQ | 79 | VAL | 2.4 |
| 24 | CC | 20 | VAL | 2.4 |
| 2 | AB | 207 | ILE | 2.4 |
| 25 | CD | 22 | ILE | 2.4 |
| 2 | AB | 65 | GLY | 2.4 |
| 3 | BC | 2 | GLY | 2.4 |
| 11 | BK | 90 | GLY | 2.4 |
| 22 | CA | 1363 | C | 2.4 |
| 22 | CA | 1909 | C | 2.4 |
| 26 | CE | 152 | GLU | 2.4 |
| 33 | CM | 138 | ALA | 2.4 |
| 34 | CN | 94 | ALA | 2.4 |
| 39 | DS | 81 | LYS | 2.4 |
| 54 | DD | 195 | GLY | 2.4 |
| 55 | DI | 14 | GLU | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 11 | BK | 56 | ARG | 2.4 |
| 44 | CX | 11 | ARG | 2.4 |
| 1 | BA | 1360 | A | 2.4 |
| 6 | BF | 58 | HIS | 2.4 |
| 22 | CA | 94 | A | 2.4 |
| 53 | DA | 279 | A | 2.4 |
| 53 | DA | 282 | A | 2.4 |
| 53 | DA | 1655 | A | 2.4 |
| 53 | DA | 2054 | A | 2.4 |
| 1 | AA | 202 | G | 2.4 |
| 1 | BA | 944 | G | 2.4 |
| 22 | CA | 1193 | G | 2.4 |
| 22 | CA | 2791 | G | 2.4 |
| 22 | CA | 2892 | G | 2.4 |
| 53 | DA | 822 | G | 2.4 |
| 53 | DA | 2004 | G | 2.4 |
| 1 | BA | 1315 | U | 2.4 |
| 23 | CB | 25 | U | 2.4 |
| 53 | DA | 360 | U | 2.4 |
| 2 | AB | 146 | ASN | 2.4 |
| 15 | AO | 69 | TYR | 2.4 |
| 18 | AR | 29 | LEU | 2.4 |
| 8 | AH | 31 | LYS | 2.4 |
| 15 | AO | 22 | THR | 2.4 |
| 21 | BU | 24 | GLU | 2.4 |
| 38 | CR | 19 | LYS | 2.4 |
| 43 | CW | 71 | LYS | 2.4 |
| 46 | DZ | 8 | GLU | 2.4 |
| 51 | C4 | 12 | LYS | 2.4 |
| 52 | C5 | 18 | LYS | 2.4 |
| 1 | BA | 222 | C | 2.4 |
| 3 | BC | 134 | MET | 2.4 |
| 16 | BP | 1 | MET | 2.4 |
| 22 | CA | 267 | C | 2.4 |
| 22 | CA | 1319 | C | 2.4 |
| 38 | DR | 37 | GLN | 2.4 |
| 53 | DA | 1656 | C | 2.4 |
| 2 | BB | 92 | VAL | 2.4 |
| 16 | AP | 78 | VAL | 2.4 |
| 33 | CM | 110 | VAL | 2.4 |
| 37 | CQ | 61 | VAL | 2.4 |
| 44 | DX | 38 | VAL | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 45 | CY | 7 | VAL | 2.4 |
| 48 | C1 | 47 | GLY | 2.4 |
| 1 | AA | 1169 | A | 2.4 |
| 1 | BA | 1329 | A | 2.4 |
| 1 | BA | 1368 | A | 2.4 |
| 22 | CA | 821 | A | 2.4 |
| 27 | DF | 2 | ALA | 2.4 |
| 24 | CC | 58 | HIS | 2.4 |
| 40 | CT | 60 | HIS | 2.4 |
| 53 | DA | 2117 | A | 2.4 |
| 53 | DA | 2134 | A | 2.4 |
| 22 | CA | 68 | G | 2.4 |
| 22 | CA | 1524 | G | 2.4 |
| 22 | CA | 1867 | G | 2.4 |
| 23 | CB | 20 | G | 2.4 |
| 2 | AB | 194 | ASP | 2.4 |
| 6 | BF | 33 | GLU | 2.4 |
| 10 | AJ | 27 | GLU | 2.4 |
| 37 | CQ | 38 | LYS | 2.4 |
| 1 | BA | 962 | C | 2.4 |
| 2 | AB | 184 | PHE | 2.4 |
| 16 | AP | 63 | GLN | 2.4 |
| 22 | CA | 1207 | C | 2.4 |
| 44 | CX | 59 | LEU | 2.4 |
| 48 | D1 | 22 | LEU | 2.4 |
| 45 | CY | 27 | ARG | 2.4 |
| 53 | DA | 2143 | C | 2.4 |
| 11 | AK | 46 | THR | 2.4 |
| 11 | BK | 96 | THR | 2.4 |
| 22 | CA | 50 | U | 2.4 |
| 26 | DE | 13 | THR | 2.4 |
| 37 | DQ | 60 | THR | 2.4 |
| 8 | BH | 53 | GLY | 2.4 |
| 8 | BH | 68 | GLY | 2.4 |
| 28 | DG | 82 | GLY | 2.4 |
| 39 | CS | 7 | SER | 2.4 |
| 22 | CA | 1525 | A | 2.4 |
| 22 | CA | 2411 | A | 2.4 |
| 31 | CK | 80 | HIS | 2.4 |
| 2 | AB | 38 | VAL | 2.4 |
| 3 | BC | 200 | VAL | 2.4 |
| 13 | AM | 64 | VAL | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 37 | CQ | 49 | ALA | 2.4 |
| 44 | DX | 18 | ALA | 2.4 |
| 55 | DI | 108 | VAL | 2.4 |
| 5 | AE | 57 | PRO | 2.4 |
| 4 | AD | 148 | LYS | 2.4 |
| 11 | BK | 109 | ASN | 2.4 |
| 34 | CN | 62 | LYS | 2.4 |
| 46 | CZ | 44 | LYS | 2.4 |
| 49 | D2 | 48 | ILE | 2.4 |
| 51 | C4 | 39 | LYS | 2.4 |
| 51 | D4 | 5 | LYS | 2.4 |
| 54 | DD | 154 | LYS | 2.4 |
| 1 | BA | 953 | G | 2.4 |
| 1 | BA | 1154 | G | 2.4 |
| 22 | CA | 245 | G | 2.4 |
| 22 | CA | 2668 | G | 2.4 |
| 53 | DA | 136 | G | 2.4 |
| 53 | DA | 533 | G | 2.4 |
| 53 | DA | 1663 | G | 2.4 |
| 3 | BC | 59 | ARG | 2.4 |
| 22 | CA | 1506 | U | 2.4 |
| 22 | CA | 246 | C | 2.4 |
| 53 | DA | 1658 | C | 2.4 |
| 1 | BA | 456 | A | 2.4 |
| 3 | BC | 23 | PHE | 2.4 |
| 3 | BC | 124 | LEU | 2.4 |
| 4 | BD | 199 | LEU | 2.4 |
| 18 | AR | 55 | LEU | 2.4 |
| 19 | AS | 63 | THR | 2.4 |
| 22 | CA | 311 | A | 2.4 |
| 22 | CA | 2657 | A | 2.4 |
| 24 | CC | 12 | GLY | 2.4 |
| 32 | DL | 32 | TYR | 2.4 |
| 33 | DM | 44 | GLY | 2.4 |
| 44 | DX | 42 | GLY | 2.4 |
| 44 | DX | 59 | LEU | 2.4 |
| 10 | AJ | 82 | LYS | 2.4 |
| 17 | AQ | 47 | HIS | 2.4 |
| 31 | CK | 132 | HIS | 2.4 |
| 40 | CT | 70 | LYS | 2.4 |
| 13 | AM | 2 | ALA | 2.3 |
| 37 | DQ | 49 | ALA | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | CA | 1181 | U | 2.3 |
| 24 | CC | 137 | VAL | 2.3 |
| 31 | CK | 105 | VAL | 2.3 |
| 33 | DM | 46 | VAL | 2.3 |
| 34 | DN | 93 | VAL | 2.3 |
| 37 | CQ | 28 | VAL | 2.3 |
| 1 | AA | 457 | G | 2.3 |
| 1 | AA | 1133 | G | 2.3 |
| 9 | BI | 80 | ARG | 2.3 |
| 14 | BN | 66 | GLN | 2.3 |
| 18 | BR | 44 | ILE | 2.3 |
| 22 | CA | 625 | G | 2.3 |
| 22 | CA | 857 | G | 2.3 |
| 22 | CA | 1163 | G | 2.3 |
| 22 | CA | 2038 | G | 2.3 |
| 32 | DL | 2 | ILE | 2.3 |
| 33 | CM | 23 | ILE | 2.3 |
| 35 | CO | 75 | ILE | 2.3 |
| 48 | C1 | 16 | ARG | 2.3 |
| 53 | DA | 2623 | G | 2.3 |
| 22 | CA | 176 | A | 2.3 |
| 22 | CA | 432 | A | 2.3 |
| 24 | CC | 41 | GLY | 2.3 |
| 26 | DE | 56 | GLY | 2.3 |
| 29 | DH | 8 | LYS | 2.3 |
| 31 | CK | 51 | GLY | 2.3 |
| 47 | D0 | 10 | THR | 2.3 |
| 50 | D3 | 1 | MET | 2.3 |
| 53 | DA | 1913 | A | 2.3 |
| 1 | AA | 5 | U | 2.3 |
| 10 | AJ | 83 | THR | 2.3 |
| 10 | AJ | 71 | LEU | 2.3 |
| 10 | BJ | 42 | LEU | 2.3 |
| 22 | CA | 2182 | U | 2.3 |
| 31 | CK | 30 | THR | 2.3 |
| 34 | DN | 95 | LEU | 2.3 |
| 48 | C1 | 6 | ASN | 2.3 |
| 53 | DA | 653 | U | 2.3 |
| 4 | AD | 29 | ASP | 2.3 |
| 10 | BJ | 19 | ASP | 2.3 |
| 29 | CH | 101 | ASP | 2.3 |
| 38 | DR | 57 | PHE | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 48 | C1 | 48 | TYR | 2.3 |
| 4 | AD | 46 | PRO | 2.3 |
| 10 | AJ | 43 | PRO | 2.3 |
| 4 | AD | 146 | ARG | 2.3 |
| 16 | BP | 27 | ALA | 2.3 |
| 29 | DH | 106 | ALA | 2.3 |
| 34 | CN | 113 | ALA | 2.3 |
| 35 | CO | 19 | ALA | 2.3 |
| 37 | CQ | 21 | ARG | 2.3 |
| 51 | D4 | 37 | ALA | 2.3 |
| 53 | DA | 2160 | C | 2.3 |
| 1 | AA | 1043 | G | 2.3 |
| 1 | BA | 849 | G | 2.3 |
| 5 | AE | 114 | VAL | 2.3 |
| 22 | CA | 375 | G | 2.3 |
| 23 | CB | 107 | G | 2.3 |
| 2 | AB | 78 | GLU | 2.3 |
| 8 | BH | 75 | ILE | 2.3 |
| 17 | AQ | 38 | ILE | 2.3 |
| 20 | AT | 67 | ILE | 2.3 |
| 25 | CD | 7 | LYS | 2.3 |
| 29 | CH | 83 | LYS | 2.3 |
| 43 | CW | 53 | LYS | 2.3 |
| 1 | BA | 1319 | A | 2.3 |
| 11 | BK | 78 | GLY | 2.3 |
| 22 | CA | 514 | A | 2.3 |
| 23 | CB | 50 | A | 2.3 |
| 35 | CO | 101 | GLY | 2.3 |
| 53 | DA | 1103 | A | 2.3 |
| 53 | DA | 2037 | A | 2.3 |
| 13 | AM | 54 | ASP | 2.3 |
| 13 | AM | 82 | ASP | 2.3 |
| 26 | CE | 65 | THR | 2.3 |
| 28 | DG | 47 | ASP | 2.3 |
| 43 | DW | 66 | ASP | 2.3 |
| 10 | BJ | 62 | ARG | 2.3 |
| 13 | AM | 87 | ARG | 2.3 |
| 24 | CC | 153 | GLN | 2.3 |
| 24 | DC | 221 | ARG | 2.3 |
| 35 | CO | 8 | ARG | 2.3 |
| 37 | CQ | 113 | ARG | 2.3 |
| 3 | BC | 115 | LEU | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 15 | BO | 85 | LEU | 2.3 |
| 31 | DK | 109 | LEU | 2.3 |
| 35 | DO | 38 | LEU | 2.3 |
| 50 | D3 | 42 | LEU | 2.3 |
| 1 | BA | 972 | C | 2.3 |
| 10 | AJ | 65 | TYR | 2.3 |
| 22 | CA | 1117 | C | 2.3 |
| 22 | CA | 1298 | C | 2.3 |
| 22 | CA | 1488 | C | 2.3 |
| 22 | CA | 1732 | C | 2.3 |
| 31 | DK | 119 | PHE | 2.3 |
| 33 | CM | 50 | PHE | 2.3 |
| 35 | CO | 67 | PHE | 2.3 |
| 41 | CU | 84 | TYR | 2.3 |
| 2 | AB | 174 | LYS | 2.3 |
| 3 | BC | 61 | ALA | 2.3 |
| 24 | DC | 111 | LYS | 2.3 |
| 26 | DE | 86 | ALA | 2.3 |
| 35 | CO | 91 | ALA | 2.3 |
| 48 | D1 | 57 | LYS | 2.3 |
| 51 | D4 | 11 | ALA | 2.3 |
| 22 | CA | 288 | U | 2.3 |
| 1 | AA | 1454 | G | 2.3 |
| 22 | CA | 70 | G | 2.3 |
| 22 | CA | 2250 | G | 2.3 |
| 22 | CA | 2732 | G | 2.3 |
| 5 | BE | 114 | VAL | 2.3 |
| 6 | AF | 89 | VAL | 2.3 |
| 19 | AS | 67 | VAL | 2.3 |
| 38 | DR | 8 | VAL | 2.3 |
| 1 | AA | 1021 | A | 2.3 |
| 4 | BD | 64 | ILE | 2.3 |
| 5 | BE | 16 | ILE | 2.3 |
| 5 | BE | 32 | SER | 2.3 |
| 24 | CC | 267 | ILE | 2.3 |
| 25 | CD | 136 | ASN | 2.3 |
| 31 | DK | 107 | GLY | 2.3 |
| 32 | CL | 95 | ILE | 2.3 |
| 35 | CO | 105 | GLY | 2.3 |
| 14 | BN | 59 | ARG | 2.3 |
| 15 | BO | 72 | ARG | 2.3 |
| 18 | BR | 48 | ARG | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 26 | CE | 170 | ARG | 2.3 |
| 31 | DK | 9 | GLU | 2.3 |
| 31 | CK | 8 | PRO | 2.3 |
| 37 | CQ | 94 | LYS | 2.3 |
| 51 | C4 | 3 | LYS | 2.3 |
| 17 | AQ | 75 | LEU | 2.3 |
| 29 | DH | 6 | LEU | 2.3 |
| 31 | DK | 36 | LEU | 2.3 |
| 2 | BB | 176 | ALA | 2.3 |
| 4 | BD | 2 | ALA | 2.3 |
| 24 | CC | 190 | ALA | 2.3 |
| 32 | CL | 79 | PHE | 2.3 |
| 33 | DM | 66 | PHE | 2.3 |
| 1 | AA | 213 | G | 2.3 |
| 1 | AA | 1006 | G | 2.3 |
| 1 | AA | 1039 | G | 2.3 |
| 1 | BA | 1231 | G | 2.3 |
| 22 | CA | 1757 | A | 2.3 |
| 22 | CA | 2371 | G | 2.3 |
| 23 | CB | 29 | A | 2.3 |
| 53 | DA | 808 | G | 2.3 |
| 2 | BB | 137 | ARG | 2.3 |
| 2 | BB | 227 | GLN | 2.3 |
| 3 | AC | 88 | ARG | 2.3 |
| 5 | BE | 148 | ASN | 2.3 |
| 12 | BL | 77 | HIS | 2.3 |
| 18 | AR | 43 | ARG | 2.3 |
| 20 | AT | 61 | GLN | 2.3 |
| 24 | CC | 38 | SER | 2.3 |
| 24 | CC | 47 | GLY | 2.3 |
| 35 | CO | 16 | HIS | 2.3 |
| 49 | D2 | 4 | GLY | 2.3 |
| 6 | AF | 98 | GLU | 2.3 |
| 15 | AO | 60 | VAL | 2.3 |
| 17 | BQ | 76 | VAL | 2.3 |
| 37 | CQ | 86 | VAL | 2.3 |
| 37 | DQ | 47 | VAL | 2.3 |
| 39 | CS | 4 | VAL | 2.3 |
| 46 | CZ | 53 | VAL | 2.3 |
| 3 | BC | 182 | ILE | 2.3 |
| 4 | AD | 177 | LYS | 2.3 |
| 5 | BE | 126 | LYS | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | CA | 2113 | U | 2.3 |
| 42 | CV | 4 | LYS | 2.3 |
| 53 | DA | 1060 | U | 2.3 |
| 1 | BA | 183 | C | 2.3 |
| 1 | BA | 848 | C | 2.3 |
| 24 | CC | 104 | ILE | 2.3 |
| 54 | DD | 123 | LYS | 2.3 |
| 26 | CE | 84 | THR | 2.3 |
| 44 | DX | 10 | THR | 2.3 |
| 12 | BL | 28 | PRO | 2.3 |
| 3 | AC | 61 | ALA | 2.3 |
| 10 | AJ | 90 | LEU | 2.3 |
| 14 | BN | 88 | ALA | 2.3 |
| 20 | AT | 37 | ALA | 2.3 |
| 26 | DE | 50 | ALA | 2.3 |
| 35 | CO | 54 | LEU | 2.3 |
| 35 | DO | 25 | ALA | 2.3 |
| 37 | CQ | 95 | ALA | 2.3 |
| 38 | DR | 63 | ALA | 2.3 |
| 55 | DI | 60 | LEU | 2.3 |
| 2 | BB | 19 | GLN | 2.3 |
| 7 | AG | 53 | ARG | 2.3 |
| 11 | BK | 64 | GLN | 2.3 |
| 27 | DF | 95 | ARG | 2.3 |
| 33 | CM | 41 | ARG | 2.3 |
| 39 | DS | 79 | ARG | 2.3 |
| 40 | CT | 11 | ARG | 2.3 |
| 48 | D1 | 13 | ARG | 2.3 |
| 53 | DA | 2033 | A | 2.3 |
| 43 | CW | 59 | GLU | 2.3 |
| 54 | DD | 124 | ARG | 2.3 |
| 2 | BB | 59 | LYS | 2.3 |
| 22 | CA | 212 | G | 2.3 |
| 15 | BO | 2 | SER | 2.3 |
| 15 | BO | 51 | HIS | 2.3 |
| 17 | BQ | 30 | LYS | 2.3 |
| 24 | DC | 240 | PHE | 2.3 |
| 24 | CC | 15 | HIS | 2.3 |
| 28 | CG | 160 | LYS | 2.3 |
| 31 | DK | 112 | GLY | 2.3 |
| 32 | CL | 81 | GLY | 2.3 |
| 33 | CM | 36 | LYS | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 37 | CQ | 87 | LYS | 2.3 |
| 38 | CR | 73 | GLY | 2.3 |
| 22 | CA | 2703 | C | 2.3 |
| 29 | DH | 121 | VAL | 2.3 |
| 37 | DQ | 26 | VAL | 2.3 |
| 52 | C5 | 11 | CYS | 2.3 |
| 3 | AC | 207 | ILE | 2.3 |
| 3 | BC | 75 | ILE | 2.3 |
| 6 | AF | 36 | ILE | 2.3 |
| 7 | BG | 93 | PRO | 2.3 |
| 12 | BL | 82 | ILE | 2.3 |
| 24 | DC | 11 | PRO | 2.3 |
| 24 | DC | 91 | ILE | 2.3 |
| 40 | DT | 96 | ILE | 2.3 |
| 51 | D4 | 32 | ILE | 2.3 |
| 2 | BB | 120 | GLN | 2.3 |
| 4 | AD | 172 | GLU | 2.3 |
| 22 | CA | 790 | U | 2.3 |
| 22 | CA | 1720 | U | 2.3 |
| 11 | BK | 98 | ARG | 2.3 |
| 25 | CD | 124 | ARG | 2.3 |
| 27 | CF | 140 | GLU | 2.3 |
| 31 | CK | 35 | ARG | 2.3 |
| 35 | CO | 49 | GLU | 2.3 |
| 1 | BA | 977 | A | 2.3 |
| 1 | BA | 1219 | A | 2.3 |
| 3 | BC | 19 | ASN | 2.3 |
| 8 | AH | 38 | ASN | 2.3 |
| 22 | CA | 156 | A | 2.3 |
| 23 | CB | 115 | A | 2.3 |
| 35 | CO | 99 | LYS | 2.3 |
| 24 | DC | 158 | ALA | 2.3 |
| 53 | DA | 2020 | A | 2.3 |
| 2 | AB | 161 | LEU | 2.3 |
| 6 | BF | 11 | HIS | 2.3 |
| 22 | CA | 319 | G | 2.2 |
| 22 | CA | 458 | G | 2.2 |
| 22 | CA | 1252 | G | 2.2 |
| 22 | CA | 1356 | G | 2.2 |
| 22 | CA | 2623 | G | 2.2 |
| 22 | CA | 2822 | G | 2.2 |
| 22 | CA | 2895 | G | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 53 | DA | 530 | G | 2.2 |
| 53 | DA | 1252 | G | 2.2 |
| 1 | BA | 1037 | C | 2.2 |
| 53 | DA | 1414 | C | 2.2 |
| 14 | AN | 20 | TYR | 2.2 |
| 24 | CC | 62 | TYR | 2.2 |
| 22 | CA | 2185 | U | 2.2 |
| 48 | D1 | 15 | MET | 2.2 |
| 5 | AE | 65 | GLU | 2.2 |
| 8 | BH | 95 | VAL | 2.2 |
| 9 | AI | 47 | VAL | 2.2 |
| 40 | CT | 52 | GLU | 2.2 |
| 2 | AB | 28 | LYS | 2.2 |
| 3 | AC | 169 | ARG | 2.2 |
| 24 | CC | 36 | LYS | 2.2 |
| 37 | CQ | 10 | GLN | 2.2 |
| 37 | CQ | 103 | ARG | 2.2 |
| 37 | CQ | 104 | THR | 2.2 |
| 54 | DD | 159 | LYS | 2.2 |
| 32 | CL | 47 | ILE | 2.2 |
| 1 | BA | 263 | A | 2.2 |
| 22 | CA | 1307 | A | 2.2 |
| 22 | CA | 1810 | A | 2.2 |
| 1 | AA | 477 | C | 2.2 |
| 1 | AA | 1397 | C | 2.2 |
| 13 | AM | 15 | ALA | 2.2 |
| 22 | CA | 22 | C | 2.2 |
| 22 | CA | 2339 | C | 2.2 |
| 24 | DC | 106 | ALA | 2.2 |
| 36 | DP | 57 | ALA | 2.2 |
| 38 | DR | 12 | ALA | 2.2 |
| 44 | CX | 42 | GLY | 2.2 |
| 1 | AA | 208 | U | 2.2 |
| 1 | BA | 971 | G | 2.2 |
| 22 | CA | 665 | U | 2.2 |
| 22 | CA | 1464 | G | 2.2 |
| 22 | CA | 2027 | G | 2.2 |
| 33 | DM | 19 | LEU | 2.2 |
| 53 | DA | 830 | G | 2.2 |
| 53 | DA | 2107 | G | 2.2 |
| 5 | BE | 14 | LYS | 2.2 |
| 11 | BK | 105 | PHE | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | BC | 72 | ARG | 2.2 |
| 9 | AI | 33 | ARG | 2.2 |
| 21 | AU | 18 | ARG | 2.2 |
| 24 | CC | 171 | TYR | 2.2 |
| 33 | DM | 21 | ARG | 2.2 |
| 39 | DS | 78 | ARG | 2.2 |
| 40 | CT | 86 | MET | 2.2 |
| 9 | BI | 107 | ASP | 2.2 |
| 1 | BA | 1227 | A | 2.2 |
| 11 | BK | 81 | ASN | 2.2 |
| 18 | BR | 40 | VAL | 2.2 |
| 32 | CL | 9 | ASN | 2.2 |
| 37 | CQ | 70 | VAL | 2.2 |
| 50 | C3 | 44 | VAL | 2.2 |
| 53 | DA | 1508 | A | 2.2 |
| 5 | AE | 134 | ILE | 2.2 |
| 6 | BF | 36 | ILE | 2.2 |
| 10 | AJ | 67 | ILE | 2.2 |
| 22 | CA | 1081 | U | 2.2 |
| 22 | CA | 1518 | C | 2.2 |
| 24 | DC | 49 | ILE | 2.2 |
| 25 | CD | 146 | ILE | 2.2 |
| 24 | DC | 41 | GLY | 2.2 |
| 26 | DE | 64 | GLY | 2.2 |
| 31 | DK | 82 | GLY | 2.2 |
| 31 | DK | 83 | GLY | 2.2 |
| 35 | DO | 16 | HIS | 2.2 |
| 47 | D0 | 14 | ILE | 2.2 |
| 53 | DA | 2022 | U | 2.2 |
| 12 | BL | 84 | GLY | 2.2 |
| 51 | C4 | 51 | SER | 2.2 |
| 5 | AE | 162 | GLU | 2.2 |
| 12 | AL | 2 | ALA | 2.2 |
| 15 | AO | 6 | GLU | 2.2 |
| 20 | AT | 45 | ALA | 2.2 |
| 35 | DO | 122 | ALA | 2.2 |
| 55 | DI | 10 | ALA | 2.2 |
| 1 | AA | 97 | G | 2.2 |
| 1 | BA | 1353 | G | 2.2 |
| 23 | CB | 116 | G | 2.2 |
| 53 | DA | 809 | G | 2.2 |
| 12 | BL | 24 | LEU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 24 | CC | 43 | ARG | 2.2 |
| 24 | CC | 110 | LEU | 2.2 |
| 24 | CC | 133 | ARG | 2.2 |
| 40 | CT | 88 | ARG | 2.2 |
| 50 | C3 | 34 | ARG | 2.2 |
| 37 | CQ | 18 | PRO | 2.2 |
| 52 | C5 | 1 | MET | 2.2 |
| 16 | AP | 16 | PHE | 2.2 |
| 24 | CC | 37 | ASN | 2.2 |
| 1 | AA | 1008 | U | 2.2 |
| 1 | BA | 981 | U | 2.2 |
| 1 | BA | 1235 | U | 2.2 |
| 1 | BA | 1251 | A | 2.2 |
| 22 | CA | 348 | A | 2.2 |
| 22 | CA | 1584 | U | 2.2 |
| 23 | CB | 87 | U | 2.2 |
| 31 | CK | 5 | THR | 2.2 |
| 1 | BA | 1045 | C | 2.2 |
| 8 | AH | 39 | VAL | 2.2 |
| 8 | BH | 43 | GLU | 2.2 |
| 22 | CA | 1541 | C | 2.2 |
| 28 | DG | 17 | VAL | 2.2 |
| 2 | AB | 115 | LYS | 2.2 |
| 31 | CK | 76 | HIS | 2.2 |
| 26 | DE | 82 | GLY | 2.2 |
| 35 | DO | 101 | GLY | 2.2 |
| 39 | CS | 71 | LYS | 2.2 |
| 48 | C1 | 11 | SER | 2.2 |
| 49 | C2 | 25 | LYS | 2.2 |
| 50 | C3 | 8 | SER | 2.2 |
| 13 | AM | 93 | ARG | 2.2 |
| 17 | BQ | 33 | ILE | 2.2 |
| 38 | DR | 28 | ARG | 2.2 |
| 40 | DT | 74 | ILE | 2.2 |
| 5 | BE | 35 | ALA | 2.2 |
| 6 | BF | 68 | GLN | 2.2 |
| 7 | BG | 100 | ALA | 2.2 |
| 41 | DU | 69 | ARG | 2.2 |
| 1 | AA | 1144 | G | 2.2 |
| 1 | BA | 987 | G | 2.2 |
| 22 | CA | 597 | G | 2.2 |
| 53 | DA | 1776 | G | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 53 | DA | 1814 | G | 2.2 |
| 24 | DC | 248 | TRP | 2.2 |
| 34 | CN | 64 | TRP | 2.2 |
| 24 | CC | 130 | LEU | 2.2 |
| 31 | CK | 25 | LEU | 2.2 |
| 38 | CR | 83 | LEU | 2.2 |
| 40 | CT | 40 | ASN | 2.2 |
| 40 | DT | 80 | PRO | 2.2 |
| 1 | AA | 1042 | A | 2.2 |
| 1 | BA | 1256 | A | 2.2 |
| 22 | CA | 227 | A | 2.2 |
| 22 | CA | 368 | A | 2.2 |
| 22 | CA | 513 | A | 2.2 |
| 53 | DA | 2003 | A | 2.2 |
| 1 | BA | 634 | C | 2.2 |
| 22 | CA | 157 | C | 2.2 |
| 22 | CA | 565 | C | 2.2 |
| 24 | DC | 219 | THR | 2.2 |
| 25 | CD | 91 | THR | 2.2 |
| 27 | DF | 155 | THR | 2.2 |
| 2 | BB | 95 | ARG | 2.2 |
| 7 | AG | 37 | SER | 2.2 |
| 9 | BI | 5 | GLN | 2.2 |
| 11 | AK | 69 | ARG | 2.2 |
| 18 | BR | 57 | ARG | 2.2 |
| 24 | CC | 259 | SER | 2.2 |
| 33 | CM | 22 | GLY | 2.2 |
| 33 | CM | 25 | SER | 2.2 |
| 42 | CV | 23 | GLY | 2.2 |
| 43 | DW | 67 | GLY | 2.2 |
| 5 | BE | 18 | VAL | 2.2 |
| 28 | DG | 113 | VAL | 2.2 |
| 47 | C0 | 57 | VAL | 2.2 |
| 51 | D4 | 58 | VAL | 2.2 |
| 53 | DA | 2189 | U | 2.2 |
| 16 | AP | 4 | ILE | 2.2 |
| 24 | DC | 116 | ILE | 2.2 |
| 24 | DC | 224 | ALA | 2.2 |
| 26 | CE | 68 | ALA | 2.2 |
| 38 | CR | 21 | ALA | 2.2 |
| 41 | CU | 38 | ALA | 2.2 |
| 43 | DW | 94 | ALA | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 45 | CY | 24 | ALA | 2.2 |
| 1 | BA | 159 | G | 2.2 |
| 11 | AK | 81 | ASN | 2.2 |
| 22 | CA | 205 | G | 2.2 |
| 22 | CA | 938 | G | 2.2 |
| 23 | CB | 13 | G | 2.2 |
| 53 | DA | 559 | G | 2.2 |
| 53 | DA | 2822 | G | 2.2 |
| 54 | DD | 126 | ASN | 2.2 |
| 1 | BA | 74 | A | 2.2 |
| 1 | BA | 1054 | C | 2.2 |
| 1 | BA | 1533 | C | 2.2 |
| 15 | BO | 73 | LYS | 2.2 |
| 17 | BQ | 66 | PRO | 2.2 |
| 22 | CA | 444 | C | 2.2 |
| 22 | CA | 1490 | A | 2.2 |
| 22 | CA | 1597 | A | 2.2 |
| 39 | CS | 81 | LYS | 2.2 |
| 39 | DS | 76 | LYS | 2.2 |
| 47 | D0 | 3[A] | LYS | 2.2 |
| 24 | DC | 225 | MET | 2.2 |
| 53 | DA | 366 | C | 2.2 |
| 53 | DA | 1997 | C | 2.2 |
| 6 | BF | 47 | LEU | 2.2 |
| 15 | BO | 57 | LEU | 2.2 |
| 17 | AQ | 8 | LEU | 2.2 |
| 51 | D4 | 44 | LEU | 2.2 |
| 10 | BJ | 50 | THR | 2.2 |
| 24 | CC | 214 | ARG | 2.2 |
| 24 | CC | 263 | THR | 2.2 |
| 24 | DC | 60 | GLN | 2.2 |
| 24 | DC | 173 | THR | 2.2 |
| 24 | CC | 196 | GLY | 2.2 |
| 25 | CD | 174 | SER | 2.2 |
| 33 | DM | 24 | GLY | 2.2 |
| 33 | DM | 42 | SER | 2.2 |
| 37 | CQ | 45 | GLY | 2.2 |
| 16 | BP | 38 | PHE | 2.2 |
| 5 | AE | 128 | TYR | 2.2 |
| 11 | AK | 18 | ASP | 2.2 |
| 11 | BK | 72 | ASP | 2.2 |
| 7 | AG | 60 | GLU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | BB | 172 | ALA | 2.2 |
| 3 | BC | 150 | LYS | 2.2 |
| 9 | AI | 16 | ALA | 2.2 |
| 16 | BP | 79 | ASN | 2.2 |
| 25 | CD | 207 | VAL | 2.2 |
| 38 | DR | 4 | VAL | 2.2 |
| 24 | DC | 155 | ALA | 2.2 |
| 31 | CK | 72 | LYS | 2.2 |
| 31 | DK | 117 | ALA | 2.2 |
| 33 | CM | 97 | ALA | 2.2 |
| 40 | CT | 64 | ALA | 2.2 |
| 44 | CX | 76 | ASN | 2.2 |
| 51 | C4 | 11 | ALA | 2.2 |
| 55 | DI | 2 | ALA | 2.2 |
| 1 | AA | 1136 | C | 2.2 |
| 22 | CA | 80 | G | 2.2 |
| 22 | CA | 165 | A | 2.2 |
| 22 | CA | 474 | G | 2.2 |
| 22 | CA | 875 | G | 2.2 |
| 22 | CA | 1167 | C | 2.2 |
| 22 | CA | 1362 | C | 2.2 |
| 22 | CA | 2852 | G | 2.2 |
| 53 | DA | 561 | G | 2.2 |
| 53 | DA | 2023 | C | 2.2 |
| 53 | DA | 2138 | G | 2.2 |
| 39 | CS | 98 | ILE | 2.2 |
| 1 | BA | 70 | U | 2.2 |
| 3 | AC | 98 | PRO | 2.2 |
| 22 | CA | 369 | U | 2.2 |
| 19 | AS | 55 | ARG | 2.1 |
| 48 | C1 | 50 | ARG | 2.1 |
| 3 | BC | 190 | HIS | 2.1 |
| 50 | D3 | 31 | LEU | 2.1 |
| 51 | C4 | 33 | LEU | 2.1 |
| 2 | BB | 153 | ASP | 2.1 |
| 10 | AJ | 78 | GLU | 2.1 |
| 24 | DC | 233 | GLY | 2.1 |
| 25 | CD | 110 | THR | 2.1 |
| 33 | DM | 32 | GLY | 2.1 |
| 34 | CN | 132 | THR | 2.1 |
| 43 | CW | 69 | GLU | 2.1 |
| 46 | CZ | 12 | GLU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 8 | BH | 50 | LYS | 2.1 |
| 11 | BK | 126 | LYS | 2.1 |
| 1 | AA | 1533 | C | 2.1 |
| 22 | CA | 264 | C | 2.1 |
| 22 | CA | 1278 | C | 2.1 |
| 22 | CA | 1559 | U | 2.1 |
| 53 | DA | 898 | C | 2.1 |
| 53 | DA | 1999 | C | 2.1 |
| 53 | DA | 2579 | C | 2.1 |
| 1 | AA | 466 | A | 2.1 |
| 3 | AC | 48 | ALA | 2.1 |
| 22 | CA | 52 | A | 2.1 |
| 22 | CA | 1877 | A | 2.1 |
| 22 | CA | 2749 | A | 2.1 |
| 28 | CG | 70 | ALA | 2.1 |
| 31 | CK | 63 | ALA | 2.1 |
| 32 | CL | 62 | VAL | 2.1 |
| 38 | DR | 2 | ALA | 2.1 |
| 41 | DU | 16 | VAL | 2.1 |
| 43 | CW | 77 | VAL | 2.1 |
| 48 | C1 | 30 | VAL | 2.1 |
| 53 | DA | 981 | A | 2.1 |
| 53 | DA | 1677 | A | 2.1 |
| 9 | AI | 49 | ARG | 2.1 |
| 10 | AJ | 99 | GLN | 2.1 |
| 22 | CA | 1 | G | 2.1 |
| 22 | CA | 553 | G | 2.1 |
| 35 | DO | 109 | PRO | 2.1 |
| 37 | CQ | 41 | GLN | 2.1 |
| 38 | DR | 30 | ARG | 2.1 |
| 53 | DA | 760 | G | 2.1 |
| 53 | DA | 2029 | G | 2.1 |
| 6 | BF | 98 | GLU | 2.1 |
| 8 | BH | 52 | GLU | 2.1 |
| 27 | DF | 26 | MET | 2.1 |
| 29 | CH | 114 | GLU | 2.1 |
| 38 | CR | 94 | ILE | 2.1 |
| 39 | CS | 41 | ILE | 2.1 |
| 28 | DG | 16 | ASP | 2.1 |
| 2 | BB | 86 | SER | 2.1 |
| 5 | BE | 92 | SER | 2.1 |
| 5 | BE | 119 | GLY | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 12 | BL | 78 | SER | 2.1 |
| 13 | AM | 99 | GLY | 2.1 |
| 14 | AN | 58 | SER | 2.1 |
| 24 | DC | 40 | SER | 2.1 |
| 26 | DE | 71 | GLY | 2.1 |
| 31 | CK | 121 | LYS | 2.1 |
| 33 | CM | 13 | LYS | 2.1 |
| 34 | CN | 5 | LYS | 2.1 |
| 44 | CX | 66 | LYS | 2.1 |
| 24 | CC | 93 | LEU | 2.1 |
| 24 | DC | 110 | LEU | 2.1 |
| 32 | DL | 8 | LEU | 2.1 |
| 50 | C3 | 24 | THR | 2.1 |
| 22 | CA | 1594 | U | 2.1 |
| 53 | DA | 2006 | C | 2.1 |
| 53 | DA | 2050 | C | 2.1 |
| 1 | BA | 174 | A | 2.1 |
| 12 | BL | 54 | ARG | 2.1 |
| 39 | CS | 21 | ARG | 2.1 |
| 45 | DY | 18 | ARG | 2.1 |
| 53 | DA | 743 | A | 2.1 |
| 53 | DA | 2602 | A | 2.1 |
| 2 | BB | 83 | ALA | 2.1 |
| 3 | BC | 141 | ALA | 2.1 |
| 16 | BP | 22 | ALA | 2.1 |
| 20 | BT | 11 | ALA | 2.1 |
| 31 | CK | 134 | ALA | 2.1 |
| 36 | CP | 79 | ALA | 2.1 |
| 55 | DI | 65 | GLU | 2.1 |
| 1 | AA | 1142 | G | 2.1 |
| 4 | AD | 173 | VAL | 2.1 |
| 5 | AE | 46 | VAL | 2.1 |
| 22 | CA | 260 | G | 2.1 |
| 22 | CA | 1910 | G | 2.1 |
| 22 | CA | 2885 | G | 2.1 |
| 25 | CD | 29 | VAL | 2.1 |
| 29 | CH | 103 | VAL | 2.1 |
| 31 | DK | 110 | PRO | 2.1 |
| 53 | DA | 1131 | G | 2.1 |
| 53 | DA | 2355 | G | 2.1 |
| 53 | DA | 2677 | G | 2.1 |
| 24 | CC | 168 | ASP | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 40 | DT | 86 | MET | 2.1 |
| 3 | AC | 55 | ILE | 2.1 |
| 5 | BE | 51 | GLY | 2.1 |
| 26 | DE | 42 | GLY | 2.1 |
| 26 | DE | 77 | ILE | 2.1 |
| 37 | DQ | 65 | SER | 2.1 |
| 1 | BA | 1129 | C | 2.1 |
| 22 | CA | 1914 | C | 2.1 |
| 22 | CA | 2805 | C | 2.1 |
| 50 | C3 | 10 | LEU | 2.1 |
| 53 | DA | 544 | C | 2.1 |
| 32 | CL | 18 | ARG | 2.1 |
| 22 | CA | 2654 | A | 2.1 |
| 49 | C2 | 7 | GLU | 2.1 |
| 53 | DA | 2051 | A | 2.1 |
| 53 | DA | 2358 | A | 2.1 |
| 26 | CE | 130 | LYS | 2.1 |
| 33 | DM | 29 | LYS | 2.1 |
| 1 | AA | 1135 | U | 2.1 |
| 1 | BA | 1121 | U | 2.1 |
| 8 | BH | 90 | ASP | 2.1 |
| 9 | BI | 121 | ALA | 2.1 |
| 12 | BL | 122 | PRO | 2.1 |
| 22 | CA | 1589 | U | 2.1 |
| 46 | CZ | 61 | ALA | 2.1 |
| 47 | D0 | 18 | PRO | 2.1 |
| 2 | BB | 94 | HIS | 2.1 |
| 3 | BC | 176 | HIS | 2.1 |
| 22 | CA | 242 | G | 2.1 |
| 22 | CA | 496 | G | 2.1 |
| 22 | CA | 498 | G | 2.1 |
| 22 | CA | 2049 | G | 2.1 |
| 23 | CB | 56 | G | 2.1 |
| 31 | DK | 74 | TYR | 2.1 |
| 53 | DA | 1299 | G | 2.1 |
| 53 | DA | 2032 | G | 2.1 |
| 5 | AE | 27 | GLY | 2.1 |
| 16 | AP | 36 | VAL | 2.1 |
| 17 | AQ | 76 | VAL | 2.1 |
| 24 | DC | 196 | GLY | 2.1 |
| 31 | CK | 22 | GLY | 2.1 |
| 32 | DL | 7 | MET | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 33 | CM | 43 | GLY | 2.1 |
| 33 | DM | 45 | GLY | 2.1 |
| 51 | D4 | 9 | GLY | 2.1 |
| 16 | BP | 26 | ASN | 2.1 |
| 16 | BP | 29 | ASN | 2.1 |
| 24 | CC | 46 | ASN | 2.1 |
| 1 | BA | 995 | C | 2.1 |
| 3 | AC | 72 | ARG | 2.1 |
| 5 | AE | 163 | GLU | 2.1 |
| 9 | AI | 119 | ARG | 2.1 |
| 10 | AJ | 7 | ARG | 2.1 |
| 21 | AU | 33 | ARG | 2.1 |
| 21 | BU | 47 | ARG | 2.1 |
| 22 | CA | 611 | C | 2.1 |
| 22 | CA | 2150 | C | 2.1 |
| 2 | BB | 171 | ILE | 2.1 |
| 16 | BP | 3 | THR | 2.1 |
| 16 | BP | 33 | ILE | 2.1 |
| 21 | AU | 44 | GLU | 2.1 |
| 28 | DG | 170 | ARG | 2.1 |
| 48 | D1 | 16 | ARG | 2.1 |
| 1 | BA | 270 | A | 2.1 |
| 22 | CA | 582 | A | 2.1 |
| 22 | CA | 1477 | A | 2.1 |
| 35 | DO | 5 | LYS | 2.1 |
| 38 | CR | 16 | LYS | 2.1 |
| 5 | AE | 11 | LEU | 2.1 |
| 48 | C1 | 28 | LEU | 2.1 |
| 39 | DS | 26 | ASP | 2.1 |
| 6 | BF | 37 | HIS | 2.1 |
| 24 | CC | 8 | PRO | 2.1 |
| 24 | DC | 58 | HIS | 2.1 |
| 40 | DT | 102 | HIS | 2.1 |
| 1 | BA | 100 | G | 2.1 |
| 22 | CA | 46 | G | 2.1 |
| 22 | CA | 1436 | G | 2.1 |
| 22 | CA | 2688 | G | 2.1 |
| 24 | CC | 186 | ALA | 2.1 |
| 51 | D4 | 27 | ALA | 2.1 |
| 53 | DA | 2428 | G | 2.1 |
| 2 | AB | 142 | GLU | 2.1 |
| 7 | AG | 55 | GLY | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 11 | AK | 109 | ASN | 2.1 |
| 25 | CD | 90 | PHE | 2.1 |
| 24 | DC | 88 | SER | 2.1 |
| 25 | CD | 161 | MET | 2.1 |
| 31 | DK | 118 | MET | 2.1 |
| 32 | CL | 100 | PHE | 2.1 |
| 54 | DD | 11 | MET | 2.1 |
| 54 | DD | 120 | GLY | 2.1 |
| 15 | BO | 64 | ARG | 2.1 |
| 33 | DM | 60 | ARG | 2.1 |
| 38 | DR | 29 | SER | 2.1 |
| 38 | DR | 58 | ARG | 2.1 |
| 45 | CY | 18 | ARG | 2.1 |
| 50 | C3 | 39 | ARG | 2.1 |
| 51 | C4 | 40 | ARG | 2.1 |
| 53 | DA | 275 | C | 2.1 |
| 53 | DA | 1727 | C | 2.1 |
| 53 | DA | 2620 | C | 2.1 |
| 53 | DA | 2824 | C | 2.1 |
| 26 | DE | 78 | TRP | 2.1 |
| 29 | CH | 37 | VAL | 2.1 |
| 34 | CN | 34 | LYS | 2.1 |
| 47 | D0 | 51 | VAL | 2.1 |
| 5 | BE | 37 | THR | 2.1 |
| 10 | BJ | 22 | THR | 2.1 |
| 15 | BO | 25 | THR | 2.1 |
| 22 | CA | 756 | A | 2.1 |
| 24 | DC | 246 | THR | 2.1 |
| 51 | C4 | 17 | THR | 2.1 |
| 53 | DA | 979 | A | 2.1 |
| 53 | DA | 1096 | A | 2.1 |
| 53 | DA | 1654 | A | 2.1 |
| 53 | DA | 1998 | A | 2.1 |
| 2 | BB | 88 | ASP | 2.1 |
| 3 | AC | 202 | ILE | 2.1 |
| 31 | CK | 103 | ILE | 2.1 |
| 37 | DQ | 48 | ILE | 2.1 |
| 24 | CC | 154 | LEU | 2.1 |
| 29 | DH | 62 | LEU | 2.1 |
| 46 | CZ | 19 | LEU | 2.1 |
| 6 | BF | 16 | GLU | 2.1 |
| 16 | BP | 41 | PRO | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 21 | BU | 2 | PRO | 2.1 |
| 33 | CM | 56 | PRO | 2.1 |
| 35 | DO | 123 | GLU | 2.1 |
| 49 | D2 | 32 | GLU | 2.1 |
| 1 | BA | 68 | G | 2.1 |
| 1 | BA | 108 | G | 2.1 |
| 1 | BA | 963 | G | 2.1 |
| 1 | BA | 1370 | G | 2.1 |
| 2 | AB | 120 | GLN | 2.1 |
| 2 | BB | 178 | ASN | 2.1 |
| 3 | BC | 143 | ARG | 2.1 |
| 5 | BE | 118 | ALA | 2.1 |
| 8 | BH | 119 | ALA | 2.1 |
| 22 | CA | 39 | G | 2.1 |
| 22 | CA | 403 | U | 2.1 |
| 22 | CA | 1492 | G | 2.1 |
| 22 | CA | 2045 | C | 2.1 |
| 22 | CA | 2876 | G | 2.1 |
| 23 | CB | 68 | C | 2.1 |
| 24 | CC | 158 | ALA | 2.1 |
| 26 | CE | 94 | GLN | 2.1 |
| 26 | DE | 68 | ALA | 2.1 |
| 31 | CK | 33 | ALA | 2.1 |
| 33 | DM | 48 | ARG | 2.1 |
| 42 | CV | 16 | GLY | 2.1 |
| 43 | CW | 52 | ALA | 2.1 |
| 46 | CZ | 48 | ARG | 2.1 |
| 33 | DM | 53 | GLY | 2.1 |
| 47 | D0 | 13 | ALA | 2.1 |
| 50 | C3 | 46 | LYS | 2.1 |
| 53 | DA | 564 | C | 2.1 |
| 53 | DA | 578 | G | 2.1 |
| 53 | DA | 879 | G | 2.1 |
| 53 | DA | 978 | G | 2.1 |
| 53 | DA | 1059 | G | 2.1 |
| 53 | DA | 1646 | C | 2.1 |
| 53 | DA | 1649 | G | 2.1 |
| 53 | DA | 1817 | G | 2.1 |
| 53 | DA | 2624 | G | 2.1 |
| 54 | DD | 196 | ALA | 2.1 |
| 14 | BN | 89 | MET | 2.1 |
| 19 | AS | 66 | MET | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 44 | DX | 45 | PHE | 2.1 |
| 49 | C2 | 20 | PHE | 2.1 |
| 22 | CA | 1640 | A | 2.1 |
| 22 | CA | 1746 | A | 2.1 |
| 53 | DA | 532 | A | 2.1 |
| 53 | DA | 572 | A | 2.1 |
| 53 | DA | 2015 | A | 2.1 |
| 7 | AG | 140 | ASP | 2.1 |
| 11 | BK | 20 | VAL | 2.1 |
| 24 | CC | 195 | VAL | 2.1 |
| 2 | AB | 52 | GLU | 2.0 |
| 27 | CF | 19 | GLU | 2.0 |
| 25 | CD | 202 | ILE | 2.0 |
| 31 | DK | 47 | HIS | 2.0 |
| 44 | CX | 37 | ILE | 2.0 |
| 10 | BJ | 5 | ARG | 2.0 |
| 48 | D1 | 19 | HIS | 2.0 |
| 32 | CL | 66 | LYS | 2.0 |
| 34 | CN | 14 | LYS | 2.0 |
| 45 | CY | 44 | LYS | 2.0 |
| 12 | AL | 7 | LEU | 2.0 |
| 12 | BL | 73 | ASN | 2.0 |
| 22 | CA | 1161 | C | 2.0 |
| 32 | DL | 123 | LEU | 2.0 |
| 38 | DR | 60 | LEU | 2.0 |
| 43 | CW | 86 | LEU | 2.0 |
| 48 | D1 | 39 | LEU | 2.0 |
| 53 | DA | 1822 | C | 2.0 |
| 33 | CM | 11 | GLY | 2.0 |
| 1 | BA | 22 | G | 2.0 |
| 1 | BA | 146 | G | 2.0 |
| 22 | CA | 301 | G | 2.0 |
| 22 | CA | 379 | G | 2.0 |
| 22 | CA | 805 | G | 2.0 |
| 22 | CA | 2379 | G | 2.0 |
| 23 | CB | 105 | G | 2.0 |
| 32 | DL | 28 | SER | 2.0 |
| 53 | DA | 1482 | G | 2.0 |
| 53 | DA | 2271 | G | 2.0 |
| 53 | DA | 2825 | G | 2.0 |
| 20 | BT | 54 | MET | 2.0 |
| 1 | BA | 465 | A | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 22 | CA | 1365 | A | 2.0 |
| 22 | CA | 1744 | A | 2.0 |
| 53 | DA | 2266 | A | 2.0 |
| 12 | BL | 76 | GLU | 2.0 |
| 26 | DE | 127 | GLU | 2.0 |
| 55 | DI | 70 | GLU | 2.0 |
| 22 | CA | 451 | U | 2.0 |
| 22 | CA | 1113 | U | 2.0 |
| 27 | DF | 99 | PHE | 2.0 |
| 31 | DK | 4 | PHE | 2.0 |
| 36 | DP | 97 | PHE | 2.0 |
| 44 | DX | 69 | PHE | 2.0 |
| 47 | D0 | 53 | PHE | 2.0 |
| 2 | AB | 46 | THR | 2.0 |
| 3 | BC | 67 | THR | 2.0 |
| 4 | BD | 67 | VAL | 2.0 |
| 8 | AH | 34 | VAL | 2.0 |
| 10 | BJ | 65 | TYR | 2.0 |
| 16 | BP | 19 | VAL | 2.0 |
| 24 | CC | 160 | THR | 2.0 |
| 25 | CD | 5 | VAL | 2.0 |
| 26 | DE | 83 | VAL | 2.0 |
| 31 | CK | 100 | VAL | 2.0 |
| 31 | DK | 105 | VAL | 2.0 |
| 32 | CL | 78 | ARG | 2.0 |
| 34 | CN | 11 | LYS | 2.0 |
| 34 | DN | 89 | VAL | 2.0 |
| 40 | DT | 45 | VAL | 2.0 |
| 43 | CW | 47 | VAL | 2.0 |
| 4 | AD | 184 | ARG | 2.0 |
| 18 | AR | 48 | ARG | 2.0 |
| 24 | CC | 258 | ARG | 2.0 |
| 20 | BT | 55 | GLN | 2.0 |
| 24 | CC | 200 | HIS | 2.0 |
| 31 | DK | 80 | HIS | 2.0 |
| 38 | CR | 37 | GLN | 2.0 |
| 1 | BA | 1284 | C | 2.0 |
| 22 | CA | 902 | C | 2.0 |
| 22 | CA | 1607 | C | 2.0 |
| 22 | CA | 1639 | C | 2.0 |
| 31 | CK | 58 | ASN | 2.0 |
| 53 | DA | 740 | C | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | BB | 104 | TRP | 2.0 |
| 6 | BF | 85 | ILE | 2.0 |
| 11 | BK | 34 | ILE | 2.0 |
| 13 | AM | 84 | GLY | 2.0 |
| 26 | DE | 54 | GLY | 2.0 |
| 37 | CQ | 50 | ILE | 2.0 |
| 2 | AB | 144 | LEU | 2.0 |
| 4 | AD | 171 | LEU | 2.0 |
| 17 | BQ | 44 | LEU | 2.0 |
| 19 | AS | 71 | LEU | 2.0 |
| 25 | CD | 138 | LEU | 2.0 |
| 54 | DD | 113 | SER | 2.0 |
| 1 | AA | 94 | G | 2.0 |
| 1 | BA | 158 | G | 2.0 |
| 1 | BA | 216 | U | 2.0 |
| 1 | BA | 1253 | G | 2.0 |
| 5 | AE | 58 | ALA | 2.0 |
| 7 | AG | 51 | ALA | 2.0 |
| 7 | BG | 74 | GLU | 2.0 |
| 13 | AM | 59 | GLU | 2.0 |
| 17 | BQ | 18 | GLU | 2.0 |
| 17 | BQ | 26 | GLU | 2.0 |
| 22 | CA | 303 | G | 2.0 |
| 22 | CA | 476 | G | 2.0 |
| 22 | CA | 1039 | A | 2.0 |
| 22 | CA | 1116 | G | 2.0 |
| 22 | CA | 1332 | G | 2.0 |
| 22 | CA | 1736 | U | 2.0 |
| 22 | CA | 1913 | A | 2.0 |
| 22 | CA | 2316 | G | 2.0 |
| 24 | DC | 92 | ALA | 2.0 |
| 35 | DO | 24 | MET | 2.0 |
| 38 | CR | 46 | ALA | 2.0 |
| 47 | D0 | 47 | MET | 2.0 |
| 53 | DA | 17 | G | 2.0 |
| 53 | DA | 574 | A | 2.0 |
| 53 | DA | 575 | A | 2.0 |
| 53 | DA | 750 | A | 2.0 |
| 53 | DA | 971 | G | 2.0 |
| 53 | DA | 2046 | G | 2.0 |
| 53 | DA | 2574 | G | 2.0 |
| 53 | DA | 2578 | G | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 33 | DM | 39 | LYS | 2.0 |
| 49 | C2 | 8 | LYS | 2.0 |
| 9 | AI | 123 | ARG | 2.0 |
| 14 | AN | 13 | ARG | 2.0 |
| 39 | CS | 84 | ARG | 2.0 |
| 11 | AK | 35 | THR | 2.0 |
| 29 | DH | 18 | GLN | 2.0 |
| 38 | CR | 44 | GLN | 2.0 |
| 17 | BQ | 28 | PHE | 2.0 |
| 24 | CC | 142 | HIS | 2.0 |
| 51 | C4 | 31 | HIS | 2.0 |
| 9 | AI | 7 | TYR | 2.0 |
| 53 | DA | 531 | C | 2.0 |
| 53 | DA | 2047 | C | 2.0 |
| 53 | DA | 2129 | C | 2.0 |
| 21 | BU | 28 | VAL | 2.0 |
| 24 | DC | 19 | VAL | 2.0 |
| 32 | CL | 10 | VAL | 2.0 |
| 24 | CC | 218 | PRO | 2.0 |
| 24 | DC | 227 | PRO | 2.0 |
| 51 | C4 | 46 | PRO | 2.0 |
| 1 | BA | 480 | U | 2.0 |
| 12 | BL | 34 | CYS | 2.0 |
| 14 | AN | 72 | GLY | 2.0 |
| 21 | AU | 8 | GLU | 2.0 |
| 22 | CA | 1443 | U | 2.0 |
| 32 | CL | 84 | CYS | 2.0 |
| 7 | AG | 33 | ASP | 2.0 |
| 7 | BG | 33 | ASP | 2.0 |
| 9 | AI | 34 | SER | 2.0 |
| 1 | AA | 1016 | A | 2.0 |
| 1 | BA | 1169 | A | 2.0 |
| 2 | AB | 66 | LYS | 2.0 |
| 8 | AH | 85 | ILE | 2.0 |
| 13 | AM | 17 | ILE | 2.0 |
| 18 | AR | 72 | ASP | 2.0 |
| 33 | CM | 40 | SER | 2.0 |
| 22 | CA | 182 | A | 2.0 |
| 30 | DJ | 129 | ILE | 2.0 |
| 37 | DQ | 96 | LYS | 2.0 |
| 53 | DA | 1269 | A | 2.0 |
| 53 | DA | 1981 | A | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|------|----------------------------|-------|
| 22 | 1MG | CA | 745 | 24/25 | 0.88 | 0.18 | - | 85,88,93,95 | 0 |
| 53 | G7M | DA | 2069 | 24/25 | 0.97 | 0.24 | - | 34,38,43,43 | 0 |
| 1 | 5MC | BA | 967 | 21/22 | 0.85 | 0.15 | - | 127,132,143,145 | 0 |
| 22 | PSU | CA | 2605 | 20/21 | 0.92 | 0.17 | - | 71,79,82,83 | 0 |
| 1 | 4OC | BA | 1402 | 22/23 | 0.90 | 0.18 | - | 82,86,90,90 | 0 |
| 1 | MA6 | BA | 1518 | 24/25 | 0.92 | 0.15 | - | 68,73,78,85 | 0 |
| 53 | H2U | DA | 2449 | 20/21 | 0.99 | 0.24 | - | 26,32,38,42 | 0 |
| 1 | G7M | AA | 527 | 24/25 | 0.94 | 0.15 | - | 64,66,70,75 | 0 |
| 1 | MA6 | BA | 1519 | 24/25 | 0.89 | 0.19 | - | 67,73,79,81 | 0 |
| 1 | 2MG | AA | 966 | 24/25 | 0.94 | 0.14 | - | 69,75,80,83 | 0 |
| 53 | PSU | DA | 2580 | 20/21 | 0.98 | 0.24 | - | 27,32,38,42 | 0 |
| 22 | 6MZ | CA | 1618 | 23/24 | 0.83 | 0.16 | - | 91,97,99,100 | 0 |
| 1 | 2MG | BA | 1516 | 24/25 | 0.85 | 0.17 | - | 67,74,79,83 | 0 |
| 1 | 2MG | AA | 1207 | 24/25 | 0.90 | 0.12 | - | 89,94,98,100 | 0 |
| 1 | UR3 | BA | 1498 | 21/22 | 0.90 | 0.17 | - | 69,76,83,83 | 0 |
| 22 | 6MZ | CA | 2030 | 23/24 | 0.77 | 0.28 | - | 93,99,101,102 | 0 |
| 53 | PSU | DA | 955 | 20/21 | 0.98 | 0.20 | - | 28,33,40,40 | 0 |
| 1 | PSU | AA | 516 | 20/21 | 0.95 | 0.11 | - | 68,75,81,81 | 0 |
| 22 | PSU | CA | 2580 | 20/21 | 0.93 | 0.15 | - | 83,88,90,92 | 0 |
| 53 | PSU | DA | 2504 | 20/21 | 0.98 | 0.21 | - | 28,36,44,45 | 0 |
| 1 | PSU | BA | 516 | 20/21 | 0.85 | 0.13 | - | 73,79,89,91 | 0 |
| 1 | 2MG | BA | 1207 | 24/25 | 0.64 | 0.18 | - | 122,126,131,131 | 0 |
| 12 | D2T | AL | 89 | 10/11 | 0.95 | 0.12 | - | 59,65,70,77 | 0 |
| 1 | 5MC | AA | 1407 | 21/22 | 0.96 | 0.12 | - | 51,59,62,63 | 0 |
| 1 | 5MC | BA | 1407 | 21/22 | 0.86 | 0.15 | - | 86,91,95,96 | 0 |
| 53 | PSU | DA | 2604 | 20/21 | 0.97 | 0.16 | - | 33,44,54,57 | 0 |
| 1 | 4OC | AA | 1402 | 22/23 | 0.96 | 0.14 | - | 59,62,68,70 | 0 |
| 22 | 5MU | CA | 747 | 21/22 | 0.88 | 0.19 | - | 82,91,96,97 | 0 |
| 22 | PSU | CA | 1911 | 20/21 | 0.78 | 0.21 | - | 103,108,113,116 | 0 |
| 53 | OMC | DA | 2498 | 21/22 | 0.97 | 0.25 | - | 28,33,38,40 | 0 |
| 53 | 5MU | DA | 747 | 21/22 | 0.97 | 0.24 | - | 27,36,43,46 | 0 |
| 22 | PSU | CA | 955 | 20/21 | 0.85 | 0.19 | - | 100,105,109,110 | 0 |
| 54 | MEQ | DD | 150[B] | 10/11 | 0.91 | 0.30 | - | 28,32,38,39 | 10 |
| 53 | 6MZ | DA | 1618 | 23/24 | 0.98 | 0.24 | - | 29,36,44,47 | 0 |
| 53 | PSU | DA | 1911 | 20/21 | 0.93 | 0.11 | - | 69,74,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|------|-----------------------------|-------|
| 53 | 5MC | DA | 1962 | 21/22 | 0.96 | 0.14 | - | 38,48,55,59 | 0 |
| 54 | MEQ | DD | 150[A] | 10/11 | 0.91 | 0.30 | - | 23,32,39,40 | 10 |
| 1 | UR3 | AA | 1498 | 21/22 | 0.96 | 0.15 | - | 50,58,65,69 | 0 |
| 53 | 2MA | DA | 2503 | 23/24 | 0.98 | 0.23 | - | 21,37,44,48 | 0 |
| 53 | PSU | DA | 2605 | 20/21 | 0.97 | 0.18 | - | 38,45,49,50 | 0 |
| 22 | 5MU | CA | 1939 | 21/22 | 0.93 | 0.14 | - | 70,78,83,83 | 0 |
| 22 | PSU | CA | 1917 | 20/21 | 0.86 | 0.11 | - | 102,107,110,112 | 0 |
| 53 | 3TD | DA | 1915 | 21/22 | 0.90 | 0.16 | - | 76,81,87,94 | 0 |
| 22 | OMC | CA | 2498 | 21/22 | 0.91 | 0.21 | - | 90,97,99,102 | 0 |
| 34 | 4D4 | DN | 81[B] | 12/13 | 0.94 | 0.23 | - | 33,36,40,41 | 9 |
| 12 | D2T | BL | 89 | 10/11 | 0.95 | 0.14 | - | 64,74,78,93 | 0 |
| 34 | 4D4 | DN | 81[A] | 12/13 | 0.94 | 0.23 | - | 33,38,42,43 | 9 |
| 22 | 2MA | CA | 2503 | 23/24 | 0.79 | 0.21 | - | 87,90,92,94 | 0 |
| 1 | MA6 | AA | 1519 | 24/25 | 0.97 | 0.14 | - | 51,56,63,67 | 0 |
| 53 | 6MZ | DA | 2030 | 23/24 | 0.98 | 0.27 | - | 22,30,36,42 | 0 |
| 22 | PSU | CA | 2504 | 20/21 | 0.89 | 0.17 | - | 83,87,90,91 | 0 |
| 22 | 5MC | CA | 1962 | 21/22 | 0.94 | 0.14 | - | 73,78,80,83 | 0 |
| 53 | 2MG | DA | 1835 | 24/25 | 0.96 | 0.16 | - | 45,50,57,57 | 0 |
| 22 | 2MG | CA | 2445 | 24/25 | 0.89 | 0.19 | - | 88,92,96,99 | 0 |
| 22 | OMU | CA | 2552 | 21/22 | 0.93 | 0.23 | - | 80,85,87,87 | 0 |
| 53 | 1MG | DA | 745 | 24/25 | 0.98 | 0.27 | - | 25,34,41,44 | 0 |
| 1 | 2MG | AA | 1516 | 24/25 | 0.96 | 0.14 | - | 47,53,60,67 | 0 |
| 53 | PSU | DA | 2457 | 20/21 | 0.98 | 0.21 | - | 31,36,43,45 | 0 |
| 22 | G7M | CA | 2069 | 24/25 | 0.86 | 0.22 | - | 88,94,96,100 | 0 |
| 53 | PSU | DA | 1917 | 20/21 | 0.91 | 0.09 | - | 63,72,79,84 | 0 |
| 53 | OMG | DA | 2251 | 24/25 | 0.97 | 0.22 | - | 23,34,41,43 | 0 |
| 1 | G7M | BA | 527 | 24/25 | 0.93 | 0.15 | - | 63,71,78,84 | 0 |
| 53 | 5MU | DA | 1939 | 21/22 | 0.97 | 0.17 | - | 36,42,45,50 | 0 |
| 22 | OMG | CA | 2251 | 24/25 | 0.86 | 0.19 | - | 85,92,95,98 | 0 |
| 1 | 5MC | AA | 967 | 21/22 | 0.92 | 0.19 | - | 70,76,83,84 | 0 |
| 1 | 2MG | BA | 966 | 24/25 | 0.83 | 0.16 | - | 128,136,145,147 | 0 |
| 53 | OMU | DA | 2552 | 21/22 | 0.98 | 0.21 | - | 35,42,46,49 | 0 |
| 22 | 2MG | CA | 1835 | 24/25 | 0.94 | 0.18 | - | 74,82,84,86 | 0 |
| 22 | 3TD | CA | 1915 | 21/22 | 0.82 | 0.30 | - | 109,112,115,116 | 0 |
| 22 | PSU | CA | 2457 | 20/21 | 0.89 | 0.18 | - | 91,97,101,102 | 0 |
| 22 | PSU | CA | 746 | 20/21 | 0.81 | 0.20 | - | 88,91,95,95 | 0 |
| 1 | MA6 | AA | 1518 | 24/25 | 0.96 | 0.15 | - | 45,54,59,64 | 0 |
| 34 | 4D4 | CN | 81 | 12/13 | 0.86 | 0.20 | - | 94,97,99,100 | 0 |
| 53 | 2MG | DA | 2445 | 24/25 | 0.98 | 0.23 | - | 23,32,38,40 | 0 |
| 53 | PSU | DA | 746 | 20/21 | 0.97 | 0.25 | - | 28,37,43,44 | 0 |

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|-------|----------------------------|-------|
| 56 | MG | DA | 3177 | 1/1 | 0.84 | 0.46 | 45.02 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3122 | 1/1 | 0.70 | 0.44 | 43.21 | 77,77,77,77 | 0 |
| 56 | MG | CA | 3025 | 1/1 | 0.84 | 0.65 | 39.26 | 92,92,92,92 | 0 |
| 58 | MPD | DA | 3205 | 8/8 | 0.81 | 0.43 | 22.02 | 58,63,68,70 | 0 |
| 56 | MG | DA | 3119 | 1/1 | 0.85 | 0.28 | 20.62 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3125 | 1/1 | 0.88 | 0.40 | 15.04 | 69,69,69,69 | 0 |
| 65 | ACY | DA | 3202 | 4/4 | 0.91 | 0.51 | 12.72 | 53,59,61,64 | 0 |
| 56 | MG | DA | 3027 | 1/1 | 0.96 | 0.34 | 11.26 | 42,42,42,42 | 0 |
| 56 | MG | AA | 1608 | 1/1 | 0.84 | 0.35 | 10.95 | 76,76,76,76 | 0 |
| 56 | MG | DA | 3022 | 1/1 | 0.81 | 0.31 | 10.20 | 40,40,40,40 | 0 |
| 56 | MG | AA | 1603 | 1/1 | 0.60 | 0.30 | 10.10 | 82,82,82,82 | 0 |
| 59 | PUT | DA | 3222 | 6/6 | 0.61 | 0.24 | 9.53 | 62,64,65,68 | 0 |
| 59 | PUT | AA | 1672 | 6/6 | 0.81 | 0.35 | 9.49 | 63,63,66,70 | 0 |
| 59 | PUT | DA | 3184 | 6/6 | 0.83 | 0.41 | 9.26 | 45,52,53,56 | 0 |
| 58 | MPD | DA | 3192 | 8/8 | 0.83 | 0.33 | 8.61 | 56,60,64,66 | 0 |
| 56 | MG | CA | 3036 | 1/1 | -0.33 | 0.38 | 8.57 | 94,94,94,94 | 0 |
| 56 | MG | AA | 1642 | 1/1 | 0.71 | 0.24 | 8.17 | 88,88,88,88 | 0 |
| 59 | PUT | DM | 201 | 6/6 | 0.91 | 0.36 | 8.09 | 46,49,53,54 | 0 |
| 56 | MG | AA | 1631 | 1/1 | 0.77 | 0.20 | 7.81 | 54,54,54,54 | 0 |
| 64 | PGE | D1 | 102 | 10/10 | 0.77 | 0.39 | 6.53 | 61,66,71,74 | 0 |
| 58 | MPD | AA | 1671 | 8/8 | 0.87 | 0.37 | 6.36 | 63,65,70,73 | 0 |
| 56 | MG | DA | 3035 | 1/1 | 0.79 | 0.40 | 6.33 | 38,38,38,38 | 0 |
| 61 | PEG | D3 | 102 | 7/7 | 0.90 | 0.29 | 6.22 | 50,54,70,71 | 0 |
| 58 | MPD | AA | 1676 | 8/8 | 0.93 | 0.24 | 6.15 | 60,66,72,76 | 0 |
| 56 | MG | DA | 3069 | 1/1 | 0.92 | 0.23 | 5.83 | 53,53,53,53 | 0 |
| 61 | PEG | DA | 3200 | 7/7 | 0.76 | 0.31 | 5.64 | 52,54,67,67 | 0 |
| 58 | MPD | DE | 301 | 8/8 | 0.78 | 0.46 | 5.38 | 57,67,76,80 | 0 |
| 56 | MG | AA | 1661 | 1/1 | 0.71 | 0.21 | 5.18 | 79,79,79,79 | 0 |
| 59 | PUT | DA | 3223 | 6/6 | 0.67 | 0.32 | 5.12 | 46,49,51,53 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 59 | PUT | DA | 3214 | 6/6 | 0.86 | 0.30 | 4.88 | 49,52,56,57 | 0 |
| 56 | MG | CB | 202 | 1/1 | 0.83 | 0.23 | 4.53 | 86,86,86,86 | 0 |
| 56 | MG | CA | 3132 | 1/1 | 0.79 | 0.31 | 4.50 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3045 | 1/1 | 0.94 | 0.24 | 3.82 | 44,44,44,44 | 0 |
| 56 | MG | CA | 3150 | 1/1 | 0.52 | 0.29 | 3.66 | 85,85,85,85 | 0 |
| 58 | MPD | DA | 3208 | 8/8 | 0.76 | 0.22 | 3.59 | 56,62,70,74 | 0 |
| 61 | PEG | DA | 3219 | 7/7 | 0.80 | 0.27 | 3.58 | 61,66,70,73 | 0 |
| 62 | SPD | DA | 3225 | 10/10 | 0.92 | 0.28 | 3.56 | 34,45,52,63 | 0 |
| 56 | MG | DA | 3006 | 1/1 | 0.93 | 0.26 | 3.32 | 43,43,43,43 | 0 |
| 56 | MG | DA | 3048 | 1/1 | 0.98 | 0.29 | 3.26 | 35,35,35,35 | 0 |
| 56 | MG | DA | 3057 | 1/1 | 0.89 | 0.26 | 3.24 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3090 | 1/1 | 0.93 | 0.29 | 3.19 | 42,42,42,42 | 0 |
| 66 | EDO | DA | 3198 | 4/4 | 0.81 | 0.32 | 3.17 | 49,53,54,55 | 0 |
| 56 | MG | DA | 3172 | 1/1 | 0.90 | 0.22 | 3.16 | 73,73,73,73 | 0 |
| 57 | PG4 | DR | 202 | 13/13 | 0.82 | 0.29 | 3.14 | 47,56,62,65 | 0 |
| 56 | MG | CA | 3005 | 1/1 | 0.72 | 0.37 | 3.14 | 96,96,96,96 | 0 |
| 56 | MG | DA | 3033 | 1/1 | 0.94 | 0.34 | 3.13 | 47,47,47,47 | 0 |
| 59 | PUT | DA | 3189 | 6/6 | 0.86 | 0.23 | 3.05 | 44,48,51,54 | 0 |
| 56 | MG | DA | 3126 | 1/1 | 0.48 | 0.23 | 3.05 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3011 | 1/1 | 0.99 | 0.36 | 2.94 | 33,33,33,33 | 0 |
| 64 | PGE | DA | 3186 | 10/10 | 0.94 | 0.23 | 2.87 | 37,42,58,59 | 0 |
| 56 | MG | BA | 1632 | 1/1 | 0.61 | 0.20 | 2.85 | 68,68,68,68 | 0 |
| 56 | MG | DA | 3064 | 1/1 | 0.94 | 0.30 | 2.84 | 41,41,41,41 | 0 |
| 60 | ZN | AB | 301 | 1/1 | 0.90 | 0.41 | 2.76 | 140,140,140,140 | 0 |
| 56 | MG | AA | 1611 | 1/1 | 0.88 | 0.23 | 2.61 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3091 | 1/1 | 0.97 | 0.30 | 2.58 | 36,36,36,36 | 0 |
| 59 | PUT | DA | 3220 | 6/6 | 0.86 | 0.24 | 2.47 | 56,58,62,67 | 0 |
| 56 | MG | DA | 3015 | 1/1 | 0.91 | 0.21 | 2.47 | 54,54,54,54 | 0 |
| 66 | EDO | D0 | 101 | 4/4 | 0.85 | 0.24 | 2.41 | 61,63,66,68 | 0 |
| 57 | PG4 | DA | 3193 | 13/13 | 0.83 | 0.25 | 2.40 | 52,56,66,66 | 0 |
| 56 | MG | DA | 3044 | 1/1 | 0.88 | 0.28 | 2.36 | 41,41,41,41 | 0 |
| 56 | MG | DA | 3108 | 1/1 | 0.99 | 0.24 | 2.28 | 38,38,38,38 | 0 |
| 62 | SPD | DA | 3187 | 10/10 | 0.96 | 0.26 | 2.28 | 36,43,46,47 | 0 |
| 56 | MG | BA | 1605 | 1/1 | 0.78 | 0.22 | 2.28 | 81,81,81,81 | 0 |
| 56 | MG | DA | 3088 | 1/1 | 0.98 | 0.29 | 2.16 | 32,32,32,32 | 0 |
| 56 | MG | AA | 1612 | 1/1 | 0.92 | 0.21 | 2.05 | 70,70,70,70 | 0 |
| 56 | MG | CA | 3002 | 1/1 | 0.66 | 0.30 | 2.02 | 91,91,91,91 | 0 |
| 56 | MG | DA | 3007 | 1/1 | 0.98 | 0.23 | 1.95 | 40,40,40,40 | 0 |
| 56 | MG | DA | 3092 | 1/1 | 0.84 | 0.28 | 1.91 | 39,39,39,39 | 0 |
| 56 | MG | DA | 3056 | 1/1 | 0.96 | 0.23 | 1.82 | 44,44,44,44 | 0 |
| 56 | MG | AA | 1649 | 1/1 | 0.92 | 0.21 | 1.79 | 64,64,64,64 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 61 | PEG | DQ | 201 | 7/7 | 0.76 | 0.24 | 1.69 | 63,70,74,76 | 0 |
| 56 | MG | AA | 1663 | 1/1 | 0.67 | 0.18 | 1.65 | 79,79,79,79 | 0 |
| 56 | MG | CA | 3129 | 1/1 | 0.90 | 0.25 | 1.63 | 84,84,84,84 | 0 |
| 56 | MG | DA | 3014 | 1/1 | 0.96 | 0.26 | 1.61 | 36,36,36,36 | 0 |
| 56 | MG | CA | 3135 | 1/1 | 0.87 | 0.23 | 1.57 | 83,83,83,83 | 0 |
| 56 | MG | BA | 1626 | 1/1 | 0.80 | 0.26 | 1.45 | 80,80,80,80 | 0 |
| 56 | MG | DA | 3010 | 1/1 | 0.93 | 0.31 | 1.42 | 37,37,37,37 | 0 |
| 56 | MG | AA | 1637 | 1/1 | 0.96 | 0.22 | 1.41 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3107 | 1/1 | 0.97 | 0.28 | 1.39 | 33,33,33,33 | 0 |
| 56 | MG | DA | 3163 | 1/1 | 0.73 | 0.17 | 1.39 | 73,73,73,73 | 0 |
| 59 | PUT | DA | 3206 | 6/6 | 0.71 | 0.18 | 1.38 | 58,61,62,63 | 0 |
| 62 | SPD | DA | 3207 | 10/10 | 0.69 | 0.21 | 1.22 | 57,63,68,70 | 0 |
| 61 | PEG | DL | 201 | 7/7 | 0.93 | 0.15 | 1.21 | 55,58,62,66 | 0 |
| 64 | PGE | D3 | 101 | 10/10 | 0.83 | 0.19 | 0.89 | 58,65,67,68 | 0 |
| 63 | 1PE | DA | 3203 | 16/16 | 0.89 | 0.24 | 0.79 | 50,55,64,65 | 0 |
| 56 | MG | DA | 3100 | 1/1 | 0.92 | 0.22 | 0.74 | 46,46,46,46 | 0 |
| 66 | EDO | D1 | 101 | 4/4 | 0.89 | 0.17 | 0.72 | 47,52,57,63 | 0 |
| 66 | EDO | DA | 3197 | 4/4 | 0.96 | 0.22 | 0.67 | 56,58,62,65 | 0 |
| 56 | MG | CA | 3088 | 1/1 | 0.92 | 0.19 | 0.58 | 68,68,68,68 | 0 |
| 56 | MG | CA | 3137 | 1/1 | 0.85 | 0.22 | 0.53 | 78,78,78,78 | 0 |
| 57 | PG4 | AA | 1670 | 13/13 | 0.88 | 0.17 | 0.52 | 52,62,68,68 | 0 |
| 56 | MG | DA | 3095 | 1/1 | 0.89 | 0.17 | 0.48 | 49,49,49,49 | 0 |
| 60 | ZN | D5 | 101 | 1/1 | 0.99 | 0.15 | 0.40 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3029 | 1/1 | 0.95 | 0.25 | 0.38 | 41,41,41,41 | 0 |
| 64 | PGE | DS | 201 | 10/10 | 0.75 | 0.18 | 0.37 | 50,56,66,68 | 0 |
| 61 | PEG | DA | 3201 | 7/7 | 0.88 | 0.23 | 0.32 | 53,56,63,66 | 0 |
| 56 | MG | DA | 3097 | 1/1 | 0.84 | 0.21 | 0.26 | 37,37,37,37 | 0 |
| 56 | MG | CA | 3060 | 1/1 | 0.80 | 0.27 | 0.20 | 93,93,93,93 | 0 |
| 57 | PG4 | DQ | 202 | 13/13 | 0.87 | 0.15 | 0.15 | 50,58,66,66 | 0 |
| 62 | SPD | DA | 3183 | 10/10 | 0.92 | 0.18 | 0.14 | 42,51,57,57 | 0 |
| 56 | MG | AA | 1648 | 1/1 | 0.89 | 0.15 | 0.12 | 56,56,56,56 | 0 |
| 56 | MG | DA | 3229 | 1/1 | 0.94 | 0.29 | 0.10 | 42,42,42,42 | 0 |
| 58 | MPD | DS | 203 | 8/8 | 0.95 | 0.25 | 0.07 | 41,45,50,53 | 0 |
| 56 | MG | DA | 3021 | 1/1 | 0.84 | 0.22 | -0.02 | 36,36,36,36 | 0 |
| 56 | MG | DA | 3082 | 1/1 | 0.96 | 0.22 | -0.02 | 49,49,49,49 | 0 |
| 59 | PUT | DA | 3195 | 6/6 | 0.82 | 0.17 | -0.03 | 39,46,50,57 | 0 |
| 56 | MG | CA | 3104 | 1/1 | 0.70 | 0.26 | -0.07 | 83,83,83,83 | 0 |
| 56 | MG | CA | 3101 | 1/1 | 0.85 | 0.22 | -0.28 | 82,82,82,82 | 0 |
| 63 | 1PE | DA | 3185 | 16/16 | 0.89 | 0.18 | -0.32 | 39,51,68,74 | 0 |
| 58 | MPD | DE | 302 | 8/8 | 0.77 | 0.23 | -0.36 | 60,65,67,67 | 0 |
| 56 | MG | DA | 3020 | 1/1 | 1.00 | 0.20 | -0.37 | 30,30,30,30 | 0 |
| 57 | PG4 | BA | 1642 | 13/13 | 0.86 | 0.17 | -0.39 | 52,61,66,69 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 61 | PEG | AL | 201 | 7/7 | 0.93 | 0.12 | -0.49 | 57,64,71,73 | 0 |
| 64 | PGE | DU | 101 | 10/10 | 0.91 | 0.13 | -0.55 | 44,60,69,71 | 0 |
| 56 | MG | CB | 201 | 1/1 | 0.64 | 0.28 | -0.58 | 91,91,91,91 | 0 |
| 56 | MG | CA | 3013 | 1/1 | 0.79 | 0.21 | -0.65 | 89,89,89,89 | 0 |
| 56 | MG | BA | 1624 | 1/1 | 0.70 | 0.41 | -0.69 | 86,86,86,86 | 0 |
| 56 | MG | CA | 3030 | 1/1 | 0.61 | 0.19 | -0.81 | 74,74,74,74 | 0 |
| 64 | PGE | DA | 3215 | 10/10 | 0.91 | 0.12 | -0.88 | 56,62,66,70 | 0 |
| 56 | MG | AA | 1668 | 1/1 | 0.97 | 0.15 | -0.93 | 60,60,60,60 | 0 |
| 57 | PG4 | DS | 202 | 13/13 | 0.87 | 0.15 | -0.95 | 42,48,56,56 | 0 |
| 64 | PGE | DA | 3204 | 10/10 | 0.90 | 0.21 | -0.98 | 53,61,69,70 | 0 |
| 59 | PUT | AA | 1673 | 6/6 | 0.83 | 0.10 | -0.98 | 63,64,68,69 | 0 |
| 56 | MG | DA | 3110 | 1/1 | 0.98 | 0.24 | -0.98 | 33,33,33,33 | 0 |
| 56 | MG | CA | 3018 | 1/1 | 0.46 | 0.17 | -1.14 | 79,79,79,79 | 0 |
| 56 | MG | AA | 1677 | 1/1 | 0.94 | 0.09 | -1.15 | 79,79,79,79 | 0 |
| 56 | MG | DB | 201 | 1/1 | 0.93 | 0.12 | -1.21 | 62,62,62,62 | 0 |
| 56 | MG | CA | 3010 | 1/1 | 0.54 | 0.19 | -1.22 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3059 | 1/1 | 0.94 | 0.22 | -1.27 | 42,42,42,42 | 0 |
| 58 | MPD | DT | 202 | 8/8 | 0.86 | 0.19 | -1.29 | 65,66,75,75 | 0 |
| 67 | GUN | DA | 3212 | 11/11 | 0.84 | 0.13 | -1.31 | 52,58,63,69 | 0 |
| 56 | MG | CA | 3122 | 1/1 | 0.71 | 0.14 | -1.44 | 85,85,85,85 | 0 |
| 56 | MG | CA | 3090 | 1/1 | 0.54 | 0.12 | -1.44 | 80,80,80,80 | 0 |
| 56 | MG | CA | 3007 | 1/1 | 0.76 | 0.17 | -1.64 | 82,82,82,82 | 0 |
| 56 | MG | CA | 3099 | 1/1 | 0.63 | 0.17 | -1.66 | 69,69,69,69 | 0 |
| 56 | MG | CA | 3019 | 1/1 | 0.57 | 0.15 | -1.67 | 81,81,81,81 | 0 |
| 56 | MG | AA | 1629 | 1/1 | 0.70 | 0.17 | -1.79 | 67,67,67,67 | 0 |
| 56 | MG | BA | 1612 | 1/1 | 0.70 | 0.10 | -1.93 | 77,77,77,77 | 0 |
| 56 | MG | AA | 1646 | 1/1 | 0.87 | 0.16 | -1.94 | 59,59,59,59 | 0 |
| 56 | MG | CA | 3136 | 1/1 | 0.76 | 0.18 | -1.96 | 87,87,87,87 | 0 |
| 60 | ZN | C5 | 101 | 1/1 | 0.92 | 0.04 | -2.01 | 117,117,117,117 | 0 |
| 56 | MG | CA | 3152 | 1/1 | 0.78 | 0.14 | -2.11 | 77,77,77,77 | 0 |
| 56 | MG | CA | 3087 | 1/1 | 0.78 | 0.12 | -2.20 | 83,83,83,83 | 0 |
| 56 | MG | AA | 1656 | 1/1 | 0.66 | 0.08 | -2.36 | 67,67,67,67 | 0 |
| 56 | MG | DA | 3149 | 1/1 | 0.90 | 0.15 | -2.37 | 62,62,62,62 | 0 |
| 56 | MG | CA | 3017 | 1/1 | 0.86 | 0.09 | -2.39 | 82,82,82,82 | 0 |
| 57 | PG4 | DA | 3217 | 13/13 | 0.87 | 0.13 | -2.40 | 57,66,72,75 | 0 |
| 56 | MG | BA | 1602 | 1/1 | 0.96 | 0.14 | -2.40 | 76,76,76,76 | 0 |
| 56 | MG | BA | 1610 | 1/1 | 0.76 | 0.09 | -2.54 | 69,69,69,69 | 0 |
| 56 | MG | CA | 3062 | 1/1 | 0.54 | 0.11 | -2.54 | 90,90,90,90 | 0 |
| 56 | MG | CA | 3038 | 1/1 | 0.86 | 0.14 | -2.58 | 78,78,78,78 | 0 |
| 56 | MG | CA | 3102 | 1/1 | 0.84 | 0.07 | -2.82 | 78,78,78,78 | 0 |
| 56 | MG | CA | 3085 | 1/1 | 0.82 | 0.13 | -2.83 | 78,78,78,78 | 0 |
| 56 | MG | CA | 3084 | 1/1 | 0.21 | 0.11 | -2.87 | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|--------|-----------------------------|-------|
| 56 | MG | AA | 1662 | 1/1 | 0.74 | 0.09 | -2.98 | 74,74,74,74 | 0 |
| 56 | MG | CA | 3021 | 1/1 | 0.62 | 0.14 | -3.03 | 93,93,93,93 | 0 |
| 56 | MG | DA | 3123 | 1/1 | 0.97 | 0.13 | -3.13 | 43,43,43,43 | 0 |
| 56 | MG | CA | 3094 | 1/1 | 0.90 | 0.07 | -3.27 | 68,68,68,68 | 0 |
| 56 | MG | CA | 3043 | 1/1 | 0.94 | 0.12 | -3.41 | 67,67,67,67 | 0 |
| 56 | MG | AA | 1639 | 1/1 | 0.90 | 0.09 | -3.43 | 79,79,79,79 | 0 |
| 56 | MG | AA | 1644 | 1/1 | 0.68 | 0.12 | -3.46 | 76,76,76,76 | 0 |
| 59 | PUT | AA | 1674 | 6/6 | 0.86 | 0.11 | -3.49 | 61,62,67,69 | 0 |
| 56 | MG | CA | 3012 | 1/1 | 0.53 | 0.09 | -3.86 | 69,69,69,69 | 0 |
| 56 | MG | CA | 3100 | 1/1 | 0.93 | 0.11 | -3.87 | 78,78,78,78 | 0 |
| 56 | MG | BA | 1615 | 1/1 | 0.95 | 0.08 | -3.92 | 62,62,62,62 | 0 |
| 56 | MG | BA | 1617 | 1/1 | 0.54 | 0.08 | -4.00 | 82,82,82,82 | 0 |
| 56 | MG | DA | 3099 | 1/1 | 0.93 | 0.15 | -4.17 | 60,60,60,60 | 0 |
| 56 | MG | DA | 3001 | 1/1 | 0.87 | 0.13 | -4.19 | 62,62,62,62 | 0 |
| 56 | MG | CA | 3078 | 1/1 | 0.64 | 0.11 | -4.38 | 85,85,85,85 | 0 |
| 56 | MG | DA | 3146 | 1/1 | 0.94 | 0.05 | -4.61 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3079 | 1/1 | 0.89 | 0.10 | -4.63 | 55,55,55,55 | 0 |
| 56 | MG | CA | 3050 | 1/1 | 0.96 | 0.07 | -4.63 | 65,65,65,65 | 0 |
| 56 | MG | CA | 3039 | 1/1 | 0.62 | 0.08 | -4.65 | 81,81,81,81 | 0 |
| 56 | MG | AA | 1643 | 1/1 | 0.93 | 0.10 | -4.66 | 66,66,66,66 | 0 |
| 56 | MG | BA | 1613 | 1/1 | 0.81 | 0.08 | -4.68 | 65,65,65,65 | 0 |
| 56 | MG | CA | 3032 | 1/1 | 0.82 | 0.07 | -4.69 | 71,71,71,71 | 0 |
| 56 | MG | CA | 3051 | 1/1 | 0.62 | 0.10 | -4.71 | 71,71,71,71 | 0 |
| 56 | MG | BA | 1614 | 1/1 | 0.81 | 0.10 | -4.78 | 77,77,77,77 | 0 |
| 56 | MG | DA | 3024 | 1/1 | 0.92 | 0.18 | -4.79 | 64,64,64,64 | 0 |
| 56 | MG | DA | 3003 | 1/1 | 0.37 | 0.09 | -4.97 | 75,75,75,75 | 0 |
| 56 | MG | CA | 3023 | 1/1 | 0.91 | 0.08 | -5.14 | 75,75,75,75 | 0 |
| 56 | MG | DA | 3134 | 1/1 | 0.98 | 0.05 | -5.51 | 65,65,65,65 | 0 |
| 56 | MG | CA | 3143 | 1/1 | 0.96 | 0.05 | -5.95 | 74,74,74,74 | 0 |
| 56 | MG | CA | 3093 | 1/1 | 0.87 | 0.06 | -6.35 | 91,91,91,91 | 0 |
| 56 | MG | AA | 1659 | 1/1 | 0.78 | 0.06 | -6.36 | 68,68,68,68 | 0 |
| 56 | MG | BA | 1601 | 1/1 | 0.70 | 0.10 | -6.39 | 78,78,78,78 | 0 |
| 56 | MG | CA | 3026 | 1/1 | 0.76 | 0.07 | -7.06 | 75,75,75,75 | 0 |
| 56 | MG | BA | 1622 | 1/1 | 0.96 | 0.11 | -7.20 | 70,70,70,70 | 0 |
| 56 | MG | DA | 3093 | 1/1 | 0.84 | 0.09 | -7.22 | 57,57,57,57 | 0 |
| 56 | MG | DA | 3061 | 1/1 | 0.67 | 0.15 | -7.67 | 60,60,60,60 | 0 |
| 56 | MG | CA | 3008 | 1/1 | 0.87 | 0.09 | -7.97 | 79,79,79,79 | 0 |
| 56 | MG | BA | 1608 | 1/1 | 0.91 | 0.04 | -8.59 | 78,78,78,78 | 0 |
| 56 | MG | DA | 3004 | 1/1 | 0.79 | 0.07 | -9.39 | 66,66,66,66 | 0 |
| 56 | MG | DA | 3025 | 1/1 | 0.94 | 0.17 | -9.61 | 41,41,41,41 | 0 |
| 56 | MG | AA | 1653 | 1/1 | 0.79 | 0.09 | -10.69 | 63,63,63,63 | 0 |
| 56 | MG | DA | 3062 | 1/1 | 0.86 | 0.15 | -12.18 | 50,50,50,50 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|------|-----------------------------|-------|
| 66 | EDO | DR | 203 | 4/4 | 0.84 | 0.20 | - | 53,54,57,60 | 0 |
| 56 | MG | BA | 1621 | 1/1 | 0.86 | 0.17 | - | 54,54,54,54 | 0 |
| 56 | MG | DA | 3078 | 1/1 | 0.95 | 0.04 | - | 72,72,72,72 | 0 |
| 56 | MG | DA | 3180 | 1/1 | 0.74 | 0.18 | - | 78,78,78,78 | 0 |
| 56 | MG | DA | 3109 | 1/1 | 0.76 | 0.64 | - | 88,88,88,88 | 0 |
| 56 | MG | AA | 1609 | 1/1 | 0.71 | 0.40 | - | 79,79,79,79 | 0 |
| 56 | MG | AA | 1628 | 1/1 | 0.82 | 0.46 | - | 80,80,80,80 | 0 |
| 56 | MG | CA | 3031 | 1/1 | 0.55 | 0.26 | - | 90,90,90,90 | 0 |
| 59 | PUT | DA | 3224 | 6/6 | 0.95 | 0.33 | - | 43,45,54,60 | 0 |
| 56 | MG | DA | 3140 | 1/1 | 0.82 | 0.45 | - | 65,65,65,65 | 0 |
| 66 | EDO | DA | 3194 | 4/4 | 0.84 | 0.27 | - | 52,52,52,58 | 0 |
| 56 | MG | CA | 3106 | 1/1 | 0.96 | 0.40 | - | 67,67,67,67 | 0 |
| 56 | MG | DB | 208 | 1/1 | 0.79 | 0.43 | - | 79,79,79,79 | 0 |
| 56 | MG | BA | 1620 | 1/1 | 0.53 | 0.08 | - | 78,78,78,78 | 0 |
| 56 | MG | DA | 3072 | 1/1 | 0.87 | 0.12 | - | 53,53,53,53 | 0 |
| 56 | MG | DA | 3058 | 1/1 | 0.88 | 0.26 | - | 38,38,38,38 | 0 |
| 56 | MG | DA | 3142 | 1/1 | 0.94 | 0.50 | - | 64,64,64,64 | 0 |
| 56 | MG | CA | 3054 | 1/1 | 0.82 | 0.13 | - | 83,83,83,83 | 0 |
| 56 | MG | CA | 3074 | 1/1 | 0.54 | 0.33 | - | 91,91,91,91 | 0 |
| 66 | EDO | DB | 210 | 4/4 | 0.77 | 0.24 | - | 65,67,68,69 | 0 |
| 56 | MG | DA | 3087 | 1/1 | 0.92 | 0.27 | - | 31,31,31,31 | 0 |
| 56 | MG | AA | 1664 | 1/1 | 0.73 | 0.10 | - | 78,78,78,78 | 0 |
| 56 | MG | DA | 3182 | 1/1 | 0.76 | 0.49 | - | 86,86,86,86 | 0 |
| 56 | MG | AA | 1625 | 1/1 | 0.87 | 0.28 | - | 70,70,70,70 | 0 |
| 56 | MG | CA | 3035 | 1/1 | 0.19 | 0.12 | - | 81,81,81,81 | 0 |
| 56 | MG | DA | 3026 | 1/1 | 0.91 | 0.30 | - | 50,50,50,50 | 0 |
| 56 | MG | DA | 3101 | 1/1 | 0.77 | 0.10 | - | 51,51,51,51 | 0 |
| 56 | MG | BA | 1603 | 1/1 | 0.87 | 0.27 | - | 83,83,83,83 | 0 |
| 65 | ACY | DA | 3191 | 4/4 | 0.89 | 0.15 | - | 48,50,52,53 | 0 |
| 56 | MG | DA | 3066 | 1/1 | 0.91 | 0.24 | - | 44,44,44,44 | 0 |
| 68 | TRS | DA | 3221 | 8/8 | 0.68 | 0.17 | - | 65,69,75,77 | 0 |
| 56 | MG | CA | 3155 | 1/1 | 0.04 | 0.35 | - | 93,93,93,93 | 0 |
| 56 | MG | DA | 3002 | 1/1 | 0.72 | 0.18 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 1631 | 1/1 | 0.76 | 0.10 | - | 76,76,76,76 | 0 |
| 56 | MG | DA | 3148 | 1/1 | 0.97 | 0.12 | - | 66,66,66,66 | 0 |
| 56 | MG | CA | 3020 | 1/1 | 0.70 | 0.25 | - | 83,83,83,83 | 0 |
| 56 | MG | DA | 3036 | 1/1 | 0.90 | 0.19 | - | 43,43,43,43 | 0 |
| 56 | MG | CA | 3042 | 1/1 | 0.59 | 0.18 | - | 70,70,70,70 | 0 |
| 56 | MG | CA | 3105 | 1/1 | 0.88 | 0.50 | - | 68,68,68,68 | 0 |
| 56 | MG | CA | 3073 | 1/1 | -0.09 | 0.41 | - | 93,93,93,93 | 0 |
| 56 | MG | CA | 3027 | 1/1 | 0.90 | 0.34 | - | 97,97,97,97 | 0 |
| 56 | MG | CA | 3115 | 1/1 | 0.91 | 0.41 | - | 73,73,73,73 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3133 | 1/1 | 0.92 | 0.20 | - | 67,67,67,67 | 0 |
| 56 | MG | CA | 3071 | 1/1 | 0.51 | 0.20 | - | 95,95,95,95 | 0 |
| 56 | MG | CA | 3117 | 1/1 | 0.94 | 0.42 | - | 79,79,79,79 | 0 |
| 56 | MG | CA | 3108 | 1/1 | 0.95 | 0.34 | - | 65,65,65,65 | 0 |
| 56 | MG | DA | 3046 | 1/1 | 0.97 | 0.21 | - | 33,33,33,33 | 0 |
| 56 | MG | AA | 1655 | 1/1 | 0.73 | 0.08 | - | 77,77,77,77 | 0 |
| 56 | MG | CA | 3024 | 1/1 | 0.91 | 0.08 | - | 75,75,75,75 | 0 |
| 56 | MG | BA | 1616 | 1/1 | 0.60 | 0.08 | - | 86,86,86,86 | 0 |
| 56 | MG | DA | 3065 | 1/1 | 0.52 | 0.15 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3174 | 1/1 | 0.84 | 0.34 | - | 77,77,77,77 | 0 |
| 56 | MG | CA | 3044 | 1/1 | 0.86 | 0.08 | - | 73,73,73,73 | 0 |
| 56 | MG | CA | 3022 | 1/1 | 0.93 | 0.31 | - | 78,78,78,78 | 0 |
| 56 | MG | DA | 3153 | 1/1 | 0.72 | 0.54 | - | 67,67,67,67 | 0 |
| 56 | MG | CA | 3142 | 1/1 | 0.87 | 0.28 | - | 69,69,69,69 | 0 |
| 56 | MG | DA | 3053 | 1/1 | 0.90 | 0.26 | - | 38,38,38,38 | 0 |
| 56 | MG | CA | 3127 | 1/1 | 0.90 | 0.19 | - | 84,84,84,84 | 0 |
| 56 | MG | BA | 1627 | 1/1 | 0.20 | 0.23 | - | 83,83,83,83 | 0 |
| 56 | MG | CB | 203 | 1/1 | 0.63 | 0.08 | - | 90,90,90,90 | 0 |
| 56 | MG | DA | 3051 | 1/1 | 0.87 | 0.14 | - | 53,53,53,53 | 0 |
| 56 | MG | DA | 3031 | 1/1 | 0.98 | 0.23 | - | 34,34,34,34 | 0 |
| 56 | MG | DA | 3113 | 1/1 | 0.90 | 0.25 | - | 38,38,38,38 | 0 |
| 56 | MG | AA | 1618 | 1/1 | 0.92 | 0.52 | - | 78,78,78,78 | 0 |
| 56 | MG | DA | 3136 | 1/1 | 0.85 | 0.38 | - | 74,74,74,74 | 0 |
| 56 | MG | CA | 3009 | 1/1 | 0.83 | 0.19 | - | 78,78,78,78 | 0 |
| 56 | MG | AA | 1605 | 1/1 | 0.92 | 0.41 | - | 76,76,76,76 | 0 |
| 56 | MG | DA | 3155 | 1/1 | 0.93 | 0.31 | - | 66,66,66,66 | 0 |
| 56 | MG | CA | 3092 | 1/1 | 0.77 | 0.13 | - | 83,83,83,83 | 0 |
| 56 | MG | AA | 1667 | 1/1 | 0.95 | 0.13 | - | 57,57,57,57 | 0 |
| 56 | MG | BA | 1635 | 1/1 | 0.78 | 0.05 | - | 72,72,72,72 | 0 |
| 56 | MG | DA | 3071 | 1/1 | 0.95 | 0.35 | - | 37,37,37,37 | 0 |
| 56 | MG | BA | 1638 | 1/1 | 0.90 | 0.25 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3139 | 1/1 | 0.87 | 0.24 | - | 57,57,57,57 | 0 |
| 56 | MG | CA | 3055 | 1/1 | 0.76 | 0.35 | - | 78,78,78,78 | 0 |
| 56 | MG | DA | 3157 | 1/1 | 0.97 | 0.19 | - | 65,65,65,65 | 0 |
| 56 | MG | CA | 3006 | 1/1 | -0.19 | 0.72 | - | 100,100,100,100 | 0 |
| 56 | MG | DA | 3039 | 1/1 | 0.99 | 0.18 | - | 39,39,39,39 | 0 |
| 56 | MG | CA | 3148 | 1/1 | 0.95 | 0.35 | - | 73,73,73,73 | 0 |
| 56 | MG | CA | 3040 | 1/1 | 0.95 | 0.13 | - | 59,59,59,59 | 0 |
| 64 | PGE | DA | 3218 | 10/10 | 0.92 | 0.14 | - | 50,55,64,68 | 0 |
| 56 | MG | DA | 3168 | 1/1 | 0.74 | 0.11 | - | 77,77,77,77 | 0 |
| 56 | MG | AA | 1654 | 1/1 | 0.59 | 0.52 | - | 91,91,91,91 | 0 |
| 56 | MG | CA | 3139 | 1/1 | 0.90 | 0.21 | - | 71,71,71,71 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3159 | 1/1 | 0.89 | 0.17 | - | 62,62,62,62 | 0 |
| 56 | MG | DA | 3137 | 1/1 | 0.74 | 0.67 | - | 56,56,56,56 | 1 |
| 56 | MG | DA | 3016 | 1/1 | 0.77 | 0.14 | - | 63,63,63,63 | 0 |
| 56 | MG | CA | 3058 | 1/1 | 0.68 | 0.09 | - | 76,76,76,76 | 0 |
| 58 | MPD | DN | 201 | 8/8 | 0.75 | 0.29 | - | 57,63,66,71 | 0 |
| 56 | MG | DA | 3118 | 1/1 | 0.86 | 0.23 | - | 79,79,79,79 | 0 |
| 56 | MG | BA | 1618 | 1/1 | 0.91 | 0.08 | - | 74,74,74,74 | 0 |
| 56 | MG | AA | 1636 | 1/1 | 0.82 | 0.13 | - | 81,81,81,81 | 0 |
| 56 | MG | DA | 3150 | 1/1 | 0.88 | 0.23 | - | 49,49,49,49 | 0 |
| 56 | MG | DB | 203 | 1/1 | 0.88 | 0.13 | - | 51,51,51,51 | 0 |
| 56 | MG | CA | 3110 | 1/1 | 0.91 | 0.41 | - | 70,70,70,70 | 0 |
| 56 | MG | DB | 205 | 1/1 | 0.91 | 0.39 | - | 74,74,74,74 | 0 |
| 56 | MG | DA | 3145 | 1/1 | 0.78 | 0.12 | - | 69,69,69,69 | 0 |
| 56 | MG | DA | 3049 | 1/1 | 0.98 | 0.24 | - | 45,45,45,45 | 0 |
| 56 | MG | DA | 3120 | 1/1 | 0.87 | 0.92 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3089 | 1/1 | 0.97 | 0.26 | - | 32,32,32,32 | 0 |
| 56 | MG | DA | 3032 | 1/1 | 0.97 | 0.29 | - | 31,31,31,31 | 0 |
| 56 | MG | CA | 3130 | 1/1 | 0.89 | 0.12 | - | 78,78,78,78 | 0 |
| 56 | MG | AA | 1623 | 1/1 | 0.59 | 0.41 | - | 71,71,71,71 | 0 |
| 56 | MG | CA | 3112 | 1/1 | 0.72 | 0.46 | - | 81,81,81,81 | 0 |
| 56 | MG | AA | 1657 | 1/1 | 0.84 | 0.13 | - | 77,77,77,77 | 0 |
| 56 | MG | BA | 1634 | 1/1 | 0.93 | 0.06 | - | 76,76,76,76 | 0 |
| 56 | MG | CA | 3015 | 1/1 | 0.87 | 0.27 | - | 76,76,76,76 | 0 |
| 56 | MG | DA | 3042 | 1/1 | 0.62 | 0.10 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3018 | 1/1 | 0.90 | 0.24 | - | 54,54,54,54 | 0 |
| 56 | MG | DA | 3005 | 1/1 | 0.88 | 0.14 | - | 72,72,72,72 | 0 |
| 56 | MG | CA | 3003 | 1/1 | 0.50 | 0.06 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3161 | 1/1 | 0.89 | 0.27 | - | 71,71,71,71 | 0 |
| 56 | MG | CA | 3056 | 1/1 | 0.84 | 0.12 | - | 75,75,75,75 | 0 |
| 56 | MG | CA | 3134 | 1/1 | 0.93 | 0.13 | - | 79,79,79,79 | 0 |
| 56 | MG | CA | 3064 | 1/1 | 0.84 | 0.16 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3170 | 1/1 | 0.73 | 0.32 | - | 66,66,66,66 | 0 |
| 56 | MG | DA | 3147 | 1/1 | 0.77 | 0.40 | - | 73,73,73,73 | 0 |
| 56 | MG | CA | 3086 | 1/1 | 0.11 | 0.17 | - | 78,78,78,78 | 0 |
| 56 | MG | BA | 1619 | 1/1 | 0.79 | 0.06 | - | 66,66,66,66 | 0 |
| 56 | MG | CA | 3149 | 1/1 | 0.92 | 0.19 | - | 69,69,69,69 | 0 |
| 56 | MG | DA | 3040 | 1/1 | 0.93 | 0.17 | - | 48,48,48,48 | 0 |
| 64 | PGE | DA | 3226 | 10/10 | 0.87 | 0.18 | - | 59,63,67,69 | 0 |
| 56 | MG | AA | 1633 | 1/1 | 0.89 | 0.12 | - | 72,72,72,72 | 0 |
| 56 | MG | AA | 1624 | 1/1 | 0.92 | 0.58 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3103 | 1/1 | 0.80 | 0.30 | - | 44,44,44,44 | 0 |
| 56 | MG | DA | 3173 | 1/1 | 0.88 | 0.26 | - | 77,77,77,77 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 1630 | 1/1 | 0.23 | 0.32 | - | 98,98,98,98 | 0 |
| 56 | MG | CA | 3091 | 1/1 | 0.80 | 0.21 | - | 77,77,77,77 | 0 |
| 56 | MG | CA | 3069 | 1/1 | 0.83 | 0.06 | - | 80,80,80,80 | 0 |
| 56 | MG | DB | 209 | 1/1 | 0.93 | 0.18 | - | 69,69,69,69 | 0 |
| 56 | MG | CA | 3133 | 1/1 | 0.95 | 0.27 | - | 75,75,75,75 | 0 |
| 56 | MG | AA | 1614 | 1/1 | 0.85 | 0.14 | - | 75,75,75,75 | 0 |
| 56 | MG | AA | 1607 | 1/1 | 0.98 | 0.29 | - | 76,76,76,76 | 0 |
| 56 | MG | CA | 3028 | 1/1 | 0.90 | 0.12 | - | 69,69,69,69 | 0 |
| 56 | MG | BA | 1628 | 1/1 | 0.91 | 0.06 | - | 74,74,74,74 | 0 |
| 56 | MG | DA | 3131 | 1/1 | 0.76 | 0.17 | - | 70,70,70,70 | 0 |
| 61 | PEG | DA | 3228 | 7/7 | 0.86 | 0.26 | - | 55,58,61,64 | 0 |
| 56 | MG | AA | 1620 | 1/1 | 0.90 | 0.58 | - | 72,72,72,72 | 0 |
| 56 | MG | DA | 3179 | 1/1 | 0.88 | 0.14 | - | 76,76,76,76 | 0 |
| 56 | MG | DA | 3019 | 1/1 | 0.94 | 0.27 | - | 34,34,34,34 | 0 |
| 56 | MG | CA | 3033 | 1/1 | 0.79 | 0.31 | - | 90,90,90,90 | 0 |
| 56 | MG | DA | 3012 | 1/1 | 0.45 | 0.23 | - | 56,56,56,56 | 0 |
| 56 | MG | CA | 3097 | 1/1 | 0.87 | 0.10 | - | 83,83,83,83 | 0 |
| 56 | MG | DA | 3028 | 1/1 | 0.84 | 0.18 | - | 49,49,49,49 | 0 |
| 56 | MG | DA | 3156 | 1/1 | 0.83 | 0.42 | - | 74,74,74,74 | 0 |
| 61 | PEG | DP | 201 | 7/7 | 0.82 | 0.14 | - | 61,65,67,67 | 0 |
| 56 | MG | DA | 3160 | 1/1 | 0.88 | 0.45 | - | 71,71,71,71 | 0 |
| 65 | ACY | DA | 3196 | 4/4 | 0.72 | 0.19 | - | 59,65,67,71 | 0 |
| 56 | MG | CA | 3037 | 1/1 | 0.11 | 0.44 | - | 102,102,102,102 | 0 |
| 56 | MG | DA | 3143 | 1/1 | 0.86 | 0.11 | - | 77,77,77,77 | 0 |
| 56 | MG | CA | 3118 | 1/1 | 0.82 | 0.22 | - | 87,87,87,87 | 0 |
| 56 | MG | BA | 1639 | 1/1 | 0.70 | 0.21 | - | 78,78,78,78 | 0 |
| 56 | MG | CA | 3098 | 1/1 | 0.45 | 0.07 | - | 89,89,89,89 | 0 |
| 56 | MG | DA | 3121 | 1/1 | 0.86 | 0.46 | - | 85,85,85,85 | 0 |
| 56 | MG | DA | 3055 | 1/1 | 0.96 | 0.19 | - | 36,36,36,36 | 0 |
| 56 | MG | DA | 3105 | 1/1 | 0.96 | 0.23 | - | 41,41,41,41 | 0 |
| 56 | MG | DB | 206 | 1/1 | 0.72 | 0.17 | - | 82,82,82,82 | 0 |
| 56 | MG | CA | 3080 | 1/1 | 0.39 | 0.17 | - | 88,88,88,88 | 0 |
| 56 | MG | CA | 3045 | 1/1 | 0.60 | 0.10 | - | 80,80,80,80 | 0 |
| 56 | MG | CA | 3114 | 1/1 | 0.88 | 0.30 | - | 68,68,68,68 | 0 |
| 56 | MG | BA | 1633 | 1/1 | 0.84 | 0.34 | - | 85,85,85,85 | 0 |
| 56 | MG | AA | 1665 | 1/1 | 0.74 | 0.04 | - | 78,78,78,78 | 0 |
| 56 | MG | CA | 3131 | 1/1 | 0.91 | 0.17 | - | 79,79,79,79 | 0 |
| 56 | MG | DA | 3181 | 1/1 | 0.87 | 0.45 | - | 79,79,79,79 | 0 |
| 56 | MG | DA | 3176 | 1/1 | 0.92 | 0.29 | - | 70,70,70,70 | 0 |
| 56 | MG | CA | 3029 | 1/1 | 0.94 | 0.12 | - | 79,79,79,79 | 0 |
| 56 | MG | AA | 1669 | 1/1 | 0.79 | 0.08 | - | 76,76,76,76 | 0 |
| 56 | MG | DA | 3129 | 1/1 | 0.46 | 0.14 | - | 70,70,70,70 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | CA | 3145 | 1/1 | 0.02 | 0.15 | - | 90,90,90,90 | 0 |
| 66 | EDO | DA | 3210 | 4/4 | 0.82 | 0.20 | - | 62,65,69,73 | 0 |
| 56 | MG | AA | 1638 | 1/1 | 0.80 | 0.17 | - | 86,86,86,86 | 0 |
| 66 | EDO | DA | 3209 | 4/4 | 0.80 | 0.29 | - | 55,59,62,67 | 0 |
| 56 | MG | BA | 1609 | 1/1 | 0.01 | 0.36 | - | 89,89,89,89 | 0 |
| 56 | MG | DA | 3083 | 1/1 | 0.90 | 0.21 | - | 50,50,50,50 | 0 |
| 56 | MG | BA | 1641 | 1/1 | 0.21 | 0.18 | - | 86,86,86,86 | 0 |
| 56 | MG | AA | 1610 | 1/1 | 0.27 | 0.48 | - | 85,85,85,85 | 0 |
| 56 | MG | AA | 1602 | 1/1 | 0.82 | 0.23 | - | 79,79,79,79 | 0 |
| 56 | MG | CA | 3076 | 1/1 | 0.67 | 0.28 | - | 83,83,83,83 | 0 |
| 56 | MG | DA | 3075 | 1/1 | 0.90 | 0.22 | - | 48,48,48,48 | 0 |
| 56 | MG | CA | 3075 | 1/1 | 0.50 | 0.18 | - | 92,92,92,92 | 0 |
| 56 | MG | CA | 3141 | 1/1 | 0.88 | 0.30 | - | 77,77,77,77 | 0 |
| 59 | PUT | DA | 3213 | 6/6 | 0.88 | 0.17 | - | 49,55,55,58 | 0 |
| 56 | MG | AA | 1604 | 1/1 | 0.70 | 0.34 | - | 73,73,73,73 | 0 |
| 56 | MG | DA | 3117 | 1/1 | 0.95 | 0.31 | - | 54,54,54,54 | 0 |
| 66 | EDO | DB | 212 | 4/4 | 0.73 | 0.21 | - | 59,60,64,64 | 0 |
| 56 | MG | CA | 3011 | 1/1 | 0.80 | 0.06 | - | 78,78,78,78 | 0 |
| 58 | MPD | DK | 201 | 8/8 | 0.84 | 0.13 | - | 60,66,71,73 | 0 |
| 56 | MG | DA | 3068 | 1/1 | 0.98 | 0.05 | - | 70,70,70,70 | 0 |
| 56 | MG | BA | 1623 | 1/1 | 0.78 | 0.55 | - | 86,86,86,86 | 0 |
| 56 | MG | DA | 3052 | 1/1 | 0.91 | 0.10 | - | 41,41,41,41 | 0 |
| 56 | MG | DA | 3151 | 1/1 | 0.80 | 0.28 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3178 | 1/1 | 0.64 | 0.09 | - | 79,79,79,79 | 0 |
| 56 | MG | DA | 3127 | 1/1 | 0.93 | 0.46 | - | 65,65,65,65 | 0 |
| 56 | MG | BA | 1636 | 1/1 | 0.84 | 0.21 | - | 83,83,83,83 | 0 |
| 56 | MG | DA | 3167 | 1/1 | 0.82 | 0.28 | - | 64,64,64,64 | 0 |
| 56 | MG | CA | 3153 | 1/1 | 0.45 | 0.23 | - | 86,86,86,86 | 0 |
| 56 | MG | CA | 3113 | 1/1 | 0.80 | 0.36 | - | 63,63,63,63 | 0 |
| 56 | MG | CA | 3083 | 1/1 | 0.44 | 0.26 | - | 93,93,93,93 | 0 |
| 56 | MG | DR | 201 | 1/1 | 0.92 | 0.77 | - | 66,66,66,66 | 0 |
| 56 | MG | AA | 1621 | 1/1 | 0.70 | 0.45 | - | 79,79,79,79 | 0 |
| 56 | MG | DA | 3104 | 1/1 | 0.89 | 0.20 | - | 44,44,44,44 | 0 |
| 58 | MPD | DA | 3190 | 8/8 | 0.88 | 0.19 | - | 55,64,69,72 | 0 |
| 56 | MG | DA | 3030 | 1/1 | 0.97 | 0.27 | - | 34,34,34,34 | 0 |
| 56 | MG | DA | 3132 | 1/1 | 0.93 | 0.21 | - | 71,71,71,71 | 0 |
| 56 | MG | AA | 1622 | 1/1 | 0.92 | 0.35 | - | 74,74,74,74 | 0 |
| 56 | MG | DA | 3037 | 1/1 | 0.96 | 0.25 | - | 37,37,37,37 | 0 |
| 56 | MG | AA | 1616 | 1/1 | 0.55 | 0.75 | - | 83,83,83,83 | 0 |
| 56 | MG | AA | 1601 | 1/1 | 0.81 | 0.31 | - | 66,66,66,66 | 0 |
| 56 | MG | BA | 1604 | 1/1 | 0.70 | 0.24 | - | 75,75,75,75 | 0 |
| 56 | MG | AA | 1635 | 1/1 | 0.93 | 0.11 | - | 74,74,74,74 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3112 | 1/1 | 0.98 | 0.25 | - | 44,44,44,44 | 0 |
| 56 | MG | CA | 3151 | 1/1 | 0.90 | 0.06 | - | 82,82,82,82 | 0 |
| 56 | MG | DA | 3106 | 1/1 | 0.83 | 0.26 | - | 44,44,44,44 | 0 |
| 56 | MG | CA | 3004 | 1/1 | 0.65 | 0.39 | - | 95,95,95,95 | 0 |
| 56 | MG | AA | 1650 | 1/1 | 0.90 | 0.03 | - | 63,63,63,63 | 0 |
| 56 | MG | DA | 3009 | 1/1 | 0.69 | 0.10 | - | 59,59,59,59 | 0 |
| 56 | MG | DA | 3063 | 1/1 | 0.90 | 0.23 | - | 42,42,42,42 | 0 |
| 56 | MG | CA | 3052 | 1/1 | 0.67 | 0.11 | - | 79,79,79,79 | 0 |
| 56 | MG | CA | 3057 | 1/1 | 0.89 | 0.10 | - | 82,82,82,82 | 0 |
| 56 | MG | CA | 3146 | 1/1 | 0.84 | 0.51 | - | 60,60,60,60 | 1 |
| 56 | MG | DA | 3111 | 1/1 | 0.77 | 0.20 | - | 61,61,61,61 | 0 |
| 56 | MG | DA | 3141 | 1/1 | 0.76 | 0.27 | - | 73,73,73,73 | 0 |
| 59 | PUT | DA | 3188 | 6/6 | 0.90 | 0.30 | - | 32,39,44,48 | 0 |
| 56 | MG | CA | 3034 | 1/1 | 0.75 | 0.06 | - | 82,82,82,82 | 0 |
| 56 | MG | DA | 3034 | 1/1 | 0.95 | 0.30 | - | 33,33,33,33 | 0 |
| 56 | MG | DA | 3060 | 1/1 | 0.52 | 0.07 | - | 77,77,77,77 | 0 |
| 56 | MG | DA | 3070 | 1/1 | 0.44 | 0.17 | - | 52,52,52,52 | 0 |
| 56 | MG | CA | 3124 | 1/1 | 0.66 | 0.15 | - | 87,87,87,87 | 0 |
| 56 | MG | DA | 3102 | 1/1 | 0.96 | 0.34 | - | 35,35,35,35 | 0 |
| 56 | MG | DA | 3041 | 1/1 | 0.43 | 0.23 | - | 50,50,50,50 | 0 |
| 56 | MG | DA | 3038 | 1/1 | 0.82 | 0.16 | - | 44,44,44,44 | 0 |
| 56 | MG | DA | 3138 | 1/1 | 0.95 | 0.24 | - | 60,60,60,60 | 0 |
| 56 | MG | CA | 3047 | 1/1 | 0.59 | 0.10 | - | 77,77,77,77 | 0 |
| 56 | MG | DA | 3084 | 1/1 | 0.95 | 0.23 | - | 48,48,48,48 | 0 |
| 56 | MG | AA | 1606 | 1/1 | 0.58 | 0.19 | - | 83,83,83,83 | 0 |
| 56 | MG | CA | 3049 | 1/1 | 0.80 | 0.15 | - | 64,64,64,64 | 0 |
| 56 | MG | CA | 3126 | 1/1 | 0.95 | 0.25 | - | 74,74,74,74 | 0 |
| 56 | MG | CA | 3061 | 1/1 | 0.69 | 0.40 | - | 86,86,86,86 | 0 |
| 56 | MG | DA | 3050 | 1/1 | 0.80 | 0.06 | - | 55,55,55,55 | 0 |
| 56 | MG | DA | 3154 | 1/1 | 0.91 | 0.37 | - | 68,68,68,68 | 0 |
| 56 | MG | DA | 3165 | 1/1 | 0.87 | 0.37 | - | 70,70,70,70 | 0 |
| 56 | MG | CA | 3072 | 1/1 | 0.66 | 0.16 | - | 92,92,92,92 | 0 |
| 56 | MG | C3 | 101 | 1/1 | -0.16 | 0.22 | - | 97,97,97,97 | 0 |
| 56 | MG | AA | 1634 | 1/1 | 0.85 | 0.07 | - | 78,78,78,78 | 0 |
| 56 | MG | BA | 1606 | 1/1 | 0.81 | 0.23 | - | 85,85,85,85 | 0 |
| 56 | MG | DA | 3085 | 1/1 | 0.82 | 0.29 | - | 44,44,44,44 | 0 |
| 56 | MG | DA | 3128 | 1/1 | 0.74 | 0.30 | - | 74,74,74,74 | 0 |
| 56 | MG | CA | 3089 | 1/1 | 0.26 | 0.17 | - | 80,80,80,80 | 0 |
| 56 | MG | AA | 1619 | 1/1 | 0.91 | 0.29 | - | 81,81,81,81 | 0 |
| 56 | MG | DA | 3162 | 1/1 | 0.89 | 0.16 | - | 69,69,69,69 | 0 |
| 56 | MG | DB | 202 | 1/1 | 0.98 | 0.21 | - | 40,40,40,40 | 0 |
| 56 | MG | CA | 3121 | 1/1 | 0.79 | 0.14 | - | 86,86,86,86 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | CA | 3140 | 1/1 | 0.57 | 0.27 | - | 76,76,76,76 | 0 |
| 56 | MG | DA | 3098 | 1/1 | 0.95 | 0.19 | - | 37,37,37,37 | 0 |
| 56 | MG | CA | 3116 | 1/1 | 0.61 | 0.41 | - | 75,75,75,75 | 0 |
| 56 | MG | DB | 204 | 1/1 | 0.89 | 0.21 | - | 57,57,57,57 | 0 |
| 56 | MG | CA | 3125 | 1/1 | 0.79 | 0.09 | - | 84,84,84,84 | 0 |
| 56 | MG | CA | 3096 | 1/1 | 0.79 | 0.10 | - | 92,92,92,92 | 0 |
| 56 | MG | DA | 3115 | 1/1 | 0.92 | 0.17 | - | 56,56,56,56 | 0 |
| 56 | MG | DA | 3081 | 1/1 | 0.95 | 0.19 | - | 52,52,52,52 | 0 |
| 56 | MG | AA | 1641 | 1/1 | 0.78 | 0.08 | - | 71,71,71,71 | 0 |
| 56 | MG | DA | 3124 | 1/1 | 0.96 | 0.51 | - | 72,72,72,72 | 0 |
| 56 | MG | CA | 3066 | 1/1 | 0.44 | 0.47 | - | 85,85,85,85 | 0 |
| 56 | MG | DA | 3169 | 1/1 | 0.89 | 0.67 | - | 77,77,77,77 | 0 |
| 56 | MG | CA | 3119 | 1/1 | 0.92 | 0.06 | - | 83,83,83,83 | 0 |
| 56 | MG | AA | 1640 | 1/1 | 0.82 | 0.21 | - | 65,65,65,65 | 0 |
| 56 | MG | CA | 3107 | 1/1 | 0.79 | 0.28 | - | 70,70,70,70 | 0 |
| 56 | MG | DA | 3086 | 1/1 | 0.96 | 0.08 | - | 40,40,40,40 | 0 |
| 56 | MG | CA | 3041 | 1/1 | 0.86 | 0.05 | - | 72,72,72,72 | 0 |
| 56 | MG | AA | 1660 | 1/1 | 0.89 | 0.34 | - | 86,86,86,86 | 0 |
| 56 | MG | CA | 3001 | 1/1 | 0.79 | 0.16 | - | 80,80,80,80 | 0 |
| 56 | MG | CA | 3138 | 1/1 | 0.67 | 0.13 | - | 80,80,80,80 | 0 |
| 56 | MG | CA | 3068 | 1/1 | 0.54 | 0.12 | - | 85,85,85,85 | 0 |
| 56 | MG | CA | 3154 | 1/1 | 0.74 | 0.17 | - | 90,90,90,90 | 0 |
| 56 | MG | CA | 3016 | 1/1 | 0.86 | 0.06 | - | 71,71,71,71 | 0 |
| 56 | MG | DA | 3073 | 1/1 | 0.96 | 0.27 | - | 38,38,38,38 | 0 |
| 56 | MG | CA | 3144 | 1/1 | 0.91 | 0.31 | - | 73,73,73,73 | 0 |
| 56 | MG | CA | 3070 | 1/1 | 0.26 | 0.23 | - | 90,90,90,90 | 0 |
| 56 | MG | CA | 3111 | 1/1 | 0.82 | 0.49 | - | 77,77,77,77 | 0 |
| 56 | MG | DA | 3152 | 1/1 | 0.89 | 0.43 | - | 65,65,65,65 | 0 |
| 56 | MG | CA | 3048 | 1/1 | 0.89 | 0.10 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 1637 | 1/1 | 0.90 | 0.24 | - | 80,80,80,80 | 0 |
| 56 | MG | DA | 3043 | 1/1 | 0.81 | 0.18 | - | 49,49,49,49 | 0 |
| 56 | MG | AA | 1632 | 1/1 | 0.74 | 0.07 | - | 79,79,79,79 | 0 |
| 61 | PEG | DA | 3227 | 7/7 | 0.68 | 0.36 | - | 57,59,71,73 | 0 |
| 58 | MPD | DA | 3211 | 8/8 | 0.87 | 0.20 | - | 54,57,64,66 | 0 |
| 56 | MG | CA | 3065 | 1/1 | 0.92 | 0.05 | - | 73,73,73,73 | 0 |
| 56 | MG | AA | 1652 | 1/1 | 0.95 | 0.25 | - | 49,49,49,49 | 0 |
| 56 | MG | AA | 1613 | 1/1 | 0.78 | 0.59 | - | 80,80,80,80 | 0 |
| 56 | MG | AA | 1666 | 1/1 | 0.91 | 0.10 | - | 73,73,73,73 | 0 |
| 56 | MG | DA | 3166 | 1/1 | 0.78 | 0.18 | - | 73,73,73,73 | 0 |
| 56 | MG | DA | 3175 | 1/1 | 0.89 | 0.21 | - | 72,72,72,72 | 0 |
| 59 | PUT | AA | 1675 | 6/6 | 0.58 | 0.18 | - | 65,66,71,72 | 0 |
| 56 | MG | CA | 3128 | 1/1 | 0.84 | 0.44 | - | 82,82,82,82 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | BA | 1607 | 1/1 | 0.63 | 0.12 | - | 84,84,84,84 | 0 |
| 56 | MG | DA | 3171 | 1/1 | 0.61 | 0.27 | - | 76,76,76,76 | 0 |
| 56 | MG | DA | 3135 | 1/1 | 0.93 | 0.11 | - | 56,56,56,56 | 0 |
| 56 | MG | AA | 1627 | 1/1 | 0.94 | 0.38 | - | 80,80,80,80 | 0 |
| 56 | MG | AA | 1617 | 1/1 | 0.59 | 0.37 | - | 82,82,82,82 | 0 |
| 56 | MG | DA | 3067 | 1/1 | 0.96 | 0.10 | - | 50,50,50,50 | 0 |
| 56 | MG | DA | 3130 | 1/1 | 0.78 | 0.69 | - | 77,77,77,77 | 0 |
| 58 | MPD | DT | 201 | 8/8 | 0.74 | 0.35 | - | 55,63,66,73 | 0 |
| 56 | MG | AA | 1651 | 1/1 | 0.83 | 0.10 | - | 69,69,69,69 | 0 |
| 56 | MG | DA | 3054 | 1/1 | 0.96 | 0.24 | - | 35,35,35,35 | 0 |
| 56 | MG | AA | 1647 | 1/1 | 0.07 | 0.13 | - | 82,82,82,82 | 0 |
| 56 | MG | DA | 3076 | 1/1 | 0.88 | 0.09 | - | 67,67,67,67 | 0 |
| 56 | MG | CA | 3082 | 1/1 | 0.62 | 0.12 | - | 79,79,79,79 | 0 |
| 56 | MG | CA | 3067 | 1/1 | 0.80 | 0.22 | - | 84,84,84,84 | 0 |
| 56 | MG | DA | 3114 | 1/1 | 0.99 | 0.19 | - | 35,35,35,35 | 0 |
| 56 | MG | DA | 3080 | 1/1 | 0.93 | 0.06 | - | 61,61,61,61 | 0 |
| 56 | MG | CA | 3077 | 1/1 | 0.82 | 0.05 | - | 83,83,83,83 | 0 |
| 56 | MG | CA | 3081 | 1/1 | 0.69 | 0.08 | - | 83,83,83,83 | 0 |
| 56 | MG | CA | 3095 | 1/1 | 0.86 | 0.20 | - | 71,71,71,71 | 0 |
| 56 | MG | CA | 3079 | 1/1 | 0.01 | 0.18 | - | 94,94,94,94 | 0 |
| 56 | MG | CA | 3120 | 1/1 | 0.91 | 0.35 | - | 74,74,74,74 | 0 |
| 56 | MG | DA | 3094 | 1/1 | 0.85 | 0.29 | - | 38,38,38,38 | 0 |
| 56 | MG | CA | 3103 | 1/1 | 0.60 | 0.06 | - | 86,86,86,86 | 0 |
| 56 | MG | DA | 3008 | 1/1 | 0.83 | 0.16 | - | 55,55,55,55 | 0 |
| 56 | MG | DA | 3023 | 1/1 | 0.98 | 0.25 | - | 41,41,41,41 | 0 |
| 61 | PEG | DA | 3199 | 7/7 | 0.84 | 0.22 | - | 49,56,67,67 | 0 |
| 56 | MG | BA | 1625 | 1/1 | 0.10 | 0.10 | - | 89,89,89,89 | 0 |
| 56 | MG | DA | 3144 | 1/1 | 0.96 | 0.10 | - | 69,69,69,69 | 0 |
| 66 | EDO | DA | 3216 | 4/4 | 0.85 | 0.22 | - | 60,61,62,67 | 0 |
| 56 | MG | AA | 1645 | 1/1 | 0.94 | 0.20 | - | 67,67,67,67 | 0 |
| 56 | MG | CA | 3063 | 1/1 | 0.82 | 0.46 | - | 93,93,93,93 | 0 |
| 56 | MG | CA | 3147 | 1/1 | 0.77 | 0.17 | - | 55,55,55,55 | 1 |
| 56 | MG | AA | 1626 | 1/1 | 0.69 | 0.20 | - | 84,84,84,84 | 0 |
| 56 | MG | BA | 1640 | 1/1 | 0.95 | 0.30 | - | 79,79,79,79 | 0 |
| 56 | MG | AA | 1615 | 1/1 | 0.90 | 0.45 | - | 74,74,74,74 | 0 |
| 56 | MG | BA | 1629 | 1/1 | 0.80 | 0.19 | - | 77,77,77,77 | 0 |
| 56 | MG | DA | 3096 | 1/1 | 0.91 | 0.22 | - | 69,69,69,69 | 0 |
| 56 | MG | BA | 1611 | 1/1 | 0.78 | 0.16 | - | 64,64,64,64 | 0 |
| 66 | EDO | DB | 211 | 4/4 | 0.64 | 0.17 | - | 68,70,71,73 | 0 |
| 56 | MG | DA | 3077 | 1/1 | 0.76 | 0.05 | - | 70,70,70,70 | 0 |
| 56 | MG | CA | 3109 | 1/1 | 0.72 | 0.37 | - | 72,72,72,72 | 0 |
| 56 | MG | CA | 3053 | 1/1 | 0.84 | 0.04 | - | 80,80,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|-----------------------------|-------|
| 56 | MG | DA | 3074 | 1/1 | 0.97 | 0.28 | - | 42,42,42,42 | 0 |
| 56 | MG | DA | 3158 | 1/1 | 0.85 | 0.10 | - | 63,63,63,63 | 0 |
| 56 | MG | AA | 1630 | 1/1 | 0.28 | 0.23 | - | 86,86,86,86 | 0 |
| 56 | MG | AA | 1658 | 1/1 | 0.53 | 0.09 | - | 70,70,70,70 | 0 |
| 56 | MG | CA | 3059 | 1/1 | 0.28 | 0.52 | - | 91,91,91,91 | 0 |
| 56 | MG | CA | 3123 | 1/1 | 0.91 | 0.15 | - | 75,75,75,75 | 0 |
| 56 | MG | CA | 3046 | 1/1 | 0.84 | 0.20 | - | 85,85,85,85 | 0 |
| 56 | MG | DA | 3013 | 1/1 | 0.81 | 0.26 | - | 52,52,52,52 | 0 |
| 56 | MG | CA | 3014 | 1/1 | 0.86 | 0.13 | - | 78,78,78,78 | 0 |
| 56 | MG | DA | 3116 | 1/1 | 0.93 | 0.11 | - | 57,57,57,57 | 0 |
| 56 | MG | DA | 3164 | 1/1 | 0.89 | 0.29 | - | 70,70,70,70 | 0 |
| 56 | MG | DB | 207 | 1/1 | 0.72 | 0.15 | - | 75,75,75,75 | 0 |
| 56 | MG | DA | 3017 | 1/1 | 0.99 | 0.26 | - | 36,36,36,36 | 0 |
| 56 | MG | DA | 3047 | 1/1 | 0.86 | 0.24 | - | 54,54,54,54 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.