



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:45 AM GMT

PDB ID : 3PU0
Title : Crystal Structure of a vesicular stomatitis virus nucleocapsid-polyC complex
Authors : Luo, M.; Green, T.J.; Rowse, M.
Deposited on : 2010-12-03
Resolution : 3.09 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

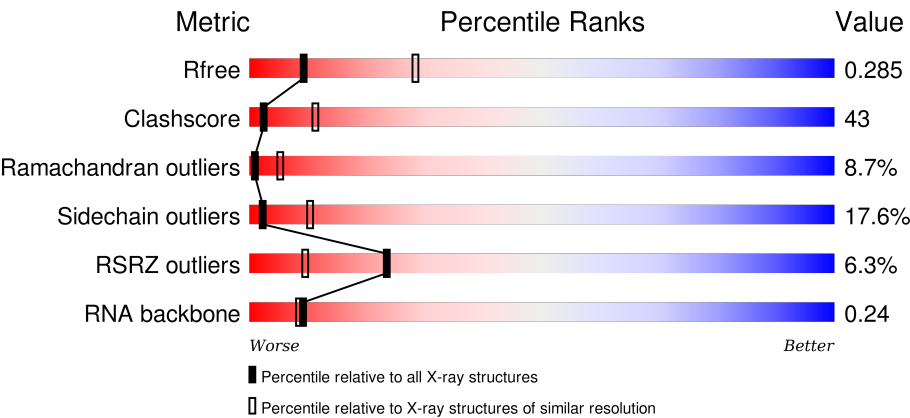
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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 | 1114 (3.14-3.06) |
| Clashscore | 102246 | 1222 (3.14-3.06) |
| Ramachandran outliers | 100387 | 1174 (3.14-3.06) |
| Sidechain outliers | 100360 | 1174 (3.14-3.06) |
| RSRZ outliers | 91569 | 1119 (3.14-3.06) |
| RNA backbone | 2183 | 1010 (3.52-2.68) |

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 | A | 421 | <div><div>8%</div><div><div></div><div>43%</div><div>43%</div><div>13%</div><div>.</div></div></div> |
| 1 | B | 421 | <div><div>3%</div><div><div></div><div>40%</div><div>43%</div><div>14%</div><div>..</div></div></div> |
| 1 | C | 421 | <div><div>5%</div><div><div></div><div>42%</div><div>40%</div><div>14%</div><div>..</div></div></div> |
| 1 | D | 421 | <div><div>6%</div><div><div></div><div>42%</div><div>42%</div><div>13%</div><div>..</div></div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | E | 421 | <div><div></div><div>9%</div><div>43%</div><div>41%</div><div>15%</div><div></div></div> |
| 2 | R | 45 | <div><div></div><div>18%</div><div>49%</div><div>29%</div><div></div></div> |

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17437 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.

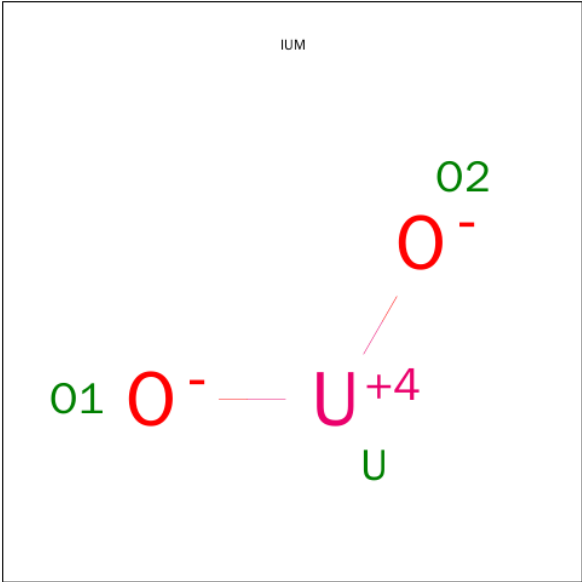
- Molecule 1 is a protein called Nucleoprotein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 421 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3327 | 2118 | 558 | 633 | 18 | | | |
| 1 | B | 415 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3290 | 2097 | 552 | 623 | 18 | | | |
| 1 | C | 413 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3275 | 2089 | 550 | 618 | 18 | | | |
| 1 | D | 416 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3298 | 2103 | 553 | 624 | 18 | | | |
| 1 | E | 421 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3327 | 2118 | 558 | 633 | 18 | | | |

- Molecule 2 is a RNA chain called RNA (45-MER).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 2 | R | 45 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 900 | 405 | 135 | 315 | 45 | | | |

- Molecule 3 is URANYL (VI) ION (three-letter code: IUM) (formula: O₂U).

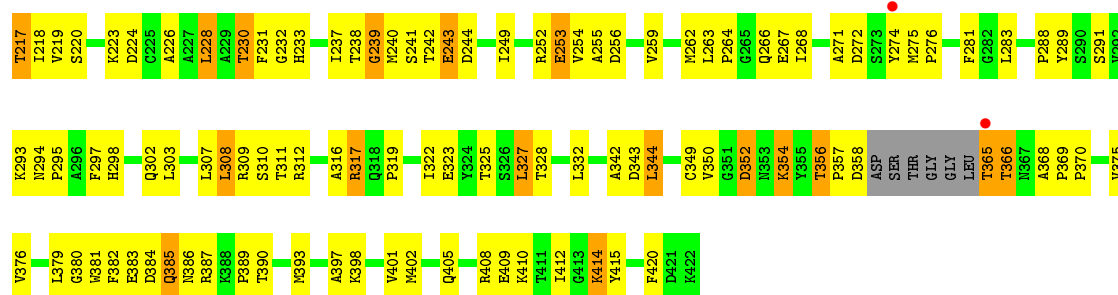


| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 3 | A | 1 | Total U 1 1 | 0 | 0 |
| 3 | A | 1 | Total U 1 1 | 0 | 0 |
| 3 | A | 1 | Total U 1 1 | 0 | 0 |
| 3 | B | 1 | Total U 1 1 | 0 | 0 |
| 3 | B | 1 | Total U 1 1 | 0 | 0 |
| 3 | B | 1 | Total U 1 1 | 0 | 0 |
| 3 | B | 1 | Total U 1 1 | 0 | 0 |
| 3 | C | 1 | Total U 1 1 | 0 | 0 |
| 3 | C | 1 | Total U 1 1 | 0 | 0 |
| 3 | D | 1 | Total U 1 1 | 0 | 0 |
| 3 | D | 1 | Total U 1 1 | 0 | 0 |
| 3 | D | 1 | Total U 1 1 | 0 | 0 |
| 3 | E | 1 | Total U 1 1 | 0 | 0 |
| 3 | E | 1 | Total U 1 1 | 0 | 0 |

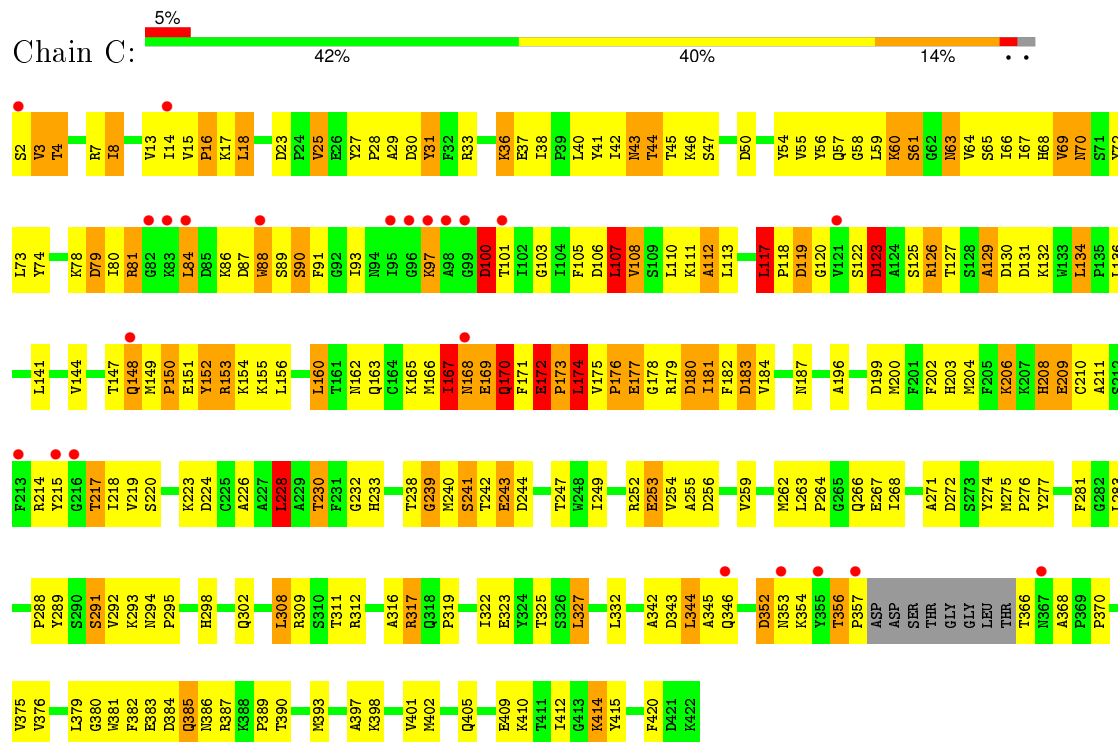
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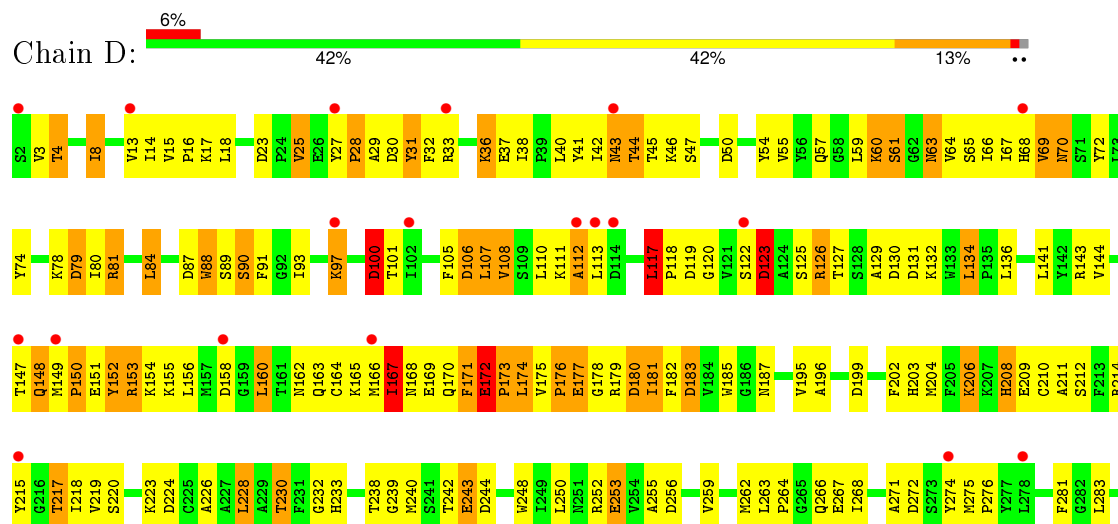
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 3 | E | 1 | Total 1 | U 1 | 0 | 0 |
| 3 | R | 1 | Total 1 | U 1 | 0 | 0 |
| 3 | R | 1 | Total 1 | U 1 | 0 | 0 |
| 3 | R | 1 | Total 1 | U 1 | 0 | 0 |
| 3 | R | 1 | Total 1 | U 1 | 0 | 0 |
| 3 | R | 1 | Total 1 | U 1 | 0 | 0 |

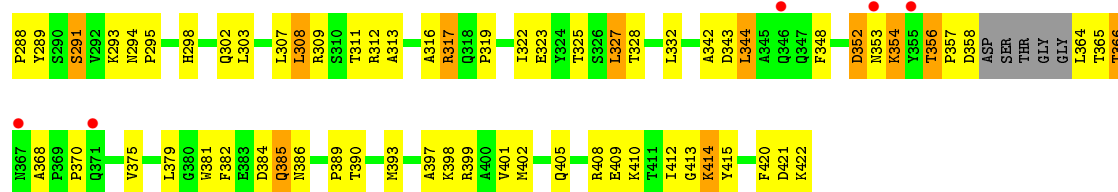


• Molecule 1: Nucleoprotein

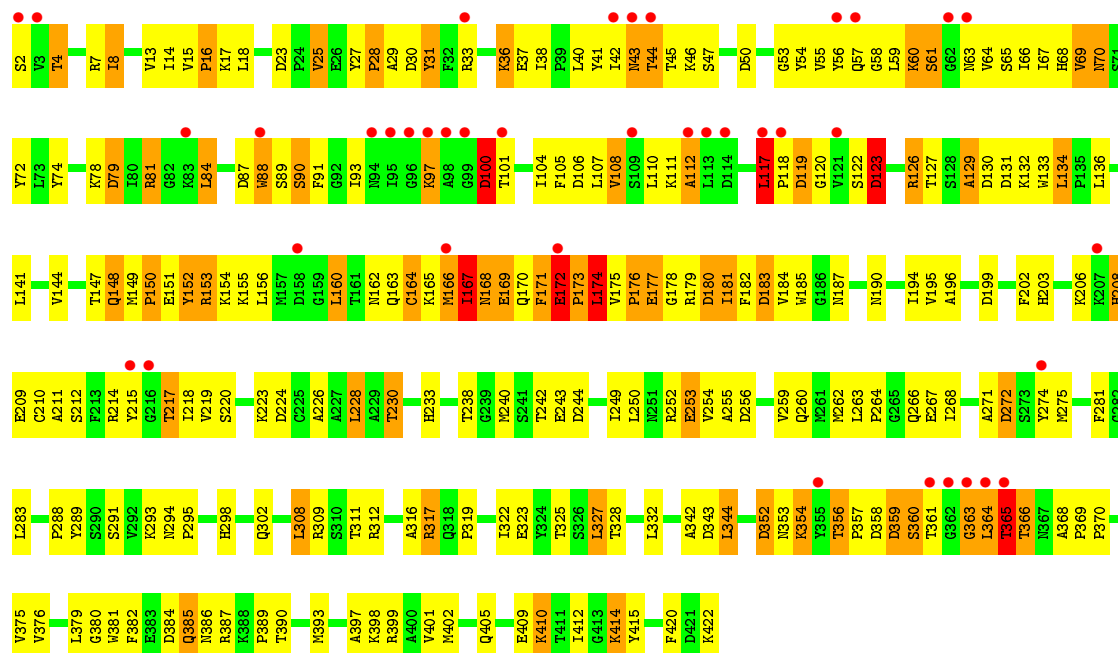


• Molecule 1: Nucleoprotein





• Molecule 1: Nucleoprotein



• Molecule 2: RNA (45-MER)



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 164.65Å 235.55Å 75.86Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.75 – 3.09 49.75 – 3.09 | Depositor EDS |
| % Data completeness (in resolution range) | 78.5 (49.75-3.09) 78.5 (49.75-3.09) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 6.16 (at 3.07Å) | Xtriage |
| Refinement program | PHENIX (PHENIX.REFINE: 1.6_289) | Depositor |
| R, R_{free} | 0.250 , 0.290 0.238 , 0.285 | Depositor DCC |
| R_{free} test set | 1885 reflections (4.33%) | DCC |
| Wilson B-factor (Å ²) | 73.2 | Xtriage |
| Anisotropy | 0.879 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.30 , 57.8 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Outliers | 1 of 46055 reflections (0.002%) | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 17437 | wwPDB-VP |
| Average B, all atoms (Å ²) | 104.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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: IUM

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 | A | 0.51 | 0/3403 | 0.67 | 1/4607 (0.0%) |
| 1 | B | 0.51 | 0/3365 | 0.65 | 1/4554 (0.0%) |
| 1 | C | 0.52 | 0/3350 | 0.65 | 0/4533 |
| 1 | D | 0.53 | 0/3373 | 0.65 | 0/4565 |
| 1 | E | 0.52 | 0/3403 | 0.66 | 0/4607 |
| 2 | R | 0.91 | 0/989 | 2.08 | 59/1526 (3.9%) |
| All | All | 0.55 | 0/17883 | 0.82 | 61/24392 (0.3%) |

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 | A | 0 | 2 |
| 1 | B | 0 | 4 |
| 1 | C | 0 | 1 |
| 1 | D | 0 | 1 |
| 1 | E | 0 | 3 |
| All | All | 0 | 11 |

There are no bond length outliers.

All (61) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|-----|------|------------|--------|------------------------|---------------------|
| 2 | R | 27 | C | O4'-C1'-N1 | 11.92 | 117.74 | 108.20 |
| 2 | R | 18 | C | N1-C1'-C2' | -11.43 | 99.14 | 114.00 |
| 2 | R | 15 | C | N1-C1'-C2' | 9.61 | 126.49 | 114.00 |
| 2 | R | 4 | C | O4'-C1'-N1 | 9.18 | 115.54 | 108.20 |
| 2 | R | 9 | C | O4'-C1'-N1 | 8.91 | 115.33 | 108.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | R | 26 | C | O4'-C1'-N1 | 8.35 | 114.88 | 108.20 |
| 2 | R | 37 | C | O4'-C1'-N1 | 7.88 | 114.50 | 108.20 |
| 2 | R | 27 | C | N1-C2-O2 | 7.78 | 123.57 | 118.90 |
| 2 | R | 41 | C | N1-C1'-C2' | -7.76 | 103.47 | 112.00 |
| 2 | R | 22 | C | O4'-C1'-N1 | 7.62 | 114.30 | 108.20 |
| 2 | R | 35 | C | O4'-C1'-N1 | 7.48 | 114.19 | 108.20 |
| 2 | R | 6 | C | C6-N1-C2 | -7.39 | 117.34 | 120.30 |
| 2 | R | 44 | C | O4'-C1'-N1 | 7.39 | 114.11 | 108.20 |
| 2 | R | 2 | C | P-O3'-C3' | -7.30 | 110.94 | 119.70 |
| 2 | R | 36 | C | O4'-C1'-N1 | 7.27 | 114.02 | 108.20 |
| 1 | A | 61 | SER | CB-CA-C | 7.21 | 123.81 | 110.10 |
| 2 | R | 4 | C | P-O3'-C3' | -7.15 | 111.12 | 119.70 |
| 2 | R | 43 | C | P-O3'-C3' | 7.06 | 128.17 | 119.70 |
| 2 | R | 30 | C | O4'-C1'-N1 | -6.95 | 102.64 | 108.20 |
| 2 | R | 9 | C | N1-C2-O2 | 6.78 | 122.97 | 118.90 |
| 2 | R | 6 | C | N1-C1'-C2' | 6.61 | 122.60 | 114.00 |
| 2 | R | 15 | C | N1-C2-O2 | 6.56 | 122.83 | 118.90 |
| 2 | R | 41 | C | C6-N1-C2 | -6.45 | 117.72 | 120.30 |
| 2 | R | 15 | C | N3-C2-O2 | -6.38 | 117.43 | 121.90 |
| 2 | R | 20 | C | P-O3'-C3' | -6.35 | 112.08 | 119.70 |
| 1 | B | 61 | SER | CB-CA-C | 6.32 | 122.11 | 110.10 |
| 2 | R | 21 | C | O4'-C1'-N1 | -6.25 | 103.20 | 108.20 |
| 2 | R | 8 | C | P-O3'-C3' | 6.23 | 127.18 | 119.70 |
| 2 | R | 25 | C | O4'-C1'-N1 | 6.20 | 113.16 | 108.20 |
| 2 | R | 10 | C | C5-C6-N1 | 6.19 | 124.10 | 121.00 |
| 2 | R | 41 | C | C3'-C2'-C1' | 6.18 | 106.45 | 101.50 |
| 2 | R | 33 | C | O4'-C1'-N1 | -6.14 | 103.29 | 108.20 |
| 2 | R | 17 | C | N1-C1'-C2' | 5.99 | 121.78 | 114.00 |
| 2 | R | 13 | C | O4'-C1'-N1 | 5.98 | 112.98 | 108.20 |
| 2 | R | 3 | C | O4'-C1'-N1 | -5.96 | 103.43 | 108.20 |
| 2 | R | 11 | C | P-O5'-C5' | 5.90 | 130.34 | 120.90 |
| 2 | R | 7 | C | O4'-C1'-N1 | -5.88 | 103.49 | 108.20 |
| 2 | R | 19 | C | P-O3'-C3' | -5.71 | 112.84 | 119.70 |
| 2 | R | 33 | C | N1-C2-O2 | 5.67 | 122.30 | 118.90 |
| 2 | R | 9 | C | N3-C2-O2 | -5.62 | 117.96 | 121.90 |
| 2 | R | 5 | C | N1-C1'-C2' | 5.57 | 121.24 | 114.00 |
| 2 | R | 1 | C | P-O3'-C3' | 5.53 | 126.33 | 119.70 |
| 2 | R | 33 | C | N1-C1'-C2' | 5.43 | 121.06 | 114.00 |
| 2 | R | 27 | C | O3'-P-O5' | -5.42 | 93.70 | 104.00 |
| 2 | R | 27 | C | C2-N1-C1' | 5.38 | 124.72 | 118.80 |
| 2 | R | 5 | C | O4'-C1'-N1 | -5.34 | 103.93 | 108.20 |
| 2 | R | 27 | C | N3-C2-O2 | -5.28 | 118.20 | 121.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | R | 4 | C | N1-C1'-C2' | 5.27 | 120.85 | 114.00 |
| 2 | R | 42 | C | N1-C1'-C2' | 5.26 | 120.84 | 114.00 |
| 2 | R | 14 | C | O4'-C1'-N1 | 5.24 | 112.39 | 108.20 |
| 2 | R | 18 | C | C3'-C2'-C1' | 5.22 | 105.68 | 101.50 |
| 2 | R | 42 | C | C6-N1-C2 | -5.20 | 118.22 | 120.30 |
| 2 | R | 30 | C | N1-C1'-C2' | 5.10 | 120.63 | 114.00 |
| 2 | R | 10 | C | O4'-C1'-N1 | -5.09 | 104.13 | 108.20 |
| 2 | R | 12 | C | N1-C1'-C2' | 5.08 | 120.61 | 114.00 |
| 2 | R | 10 | C | C2-N1-C1' | 5.08 | 124.39 | 118.80 |
| 2 | R | 33 | C | C2-N1-C1' | 5.07 | 124.38 | 118.80 |
| 2 | R | 40 | C | OP2-P-O3' | -5.06 | 94.06 | 105.20 |
| 2 | R | 21 | C | P-O3'-C3' | 5.04 | 125.75 | 119.70 |
| 2 | R | 10 | C | N3-C4-N4 | 5.04 | 121.53 | 118.00 |
| 2 | R | 40 | C | N1-C1'-C2' | 5.00 | 120.50 | 114.00 |

There are no chirality outliers.

All (11) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | A | 169 | GLU | Peptide |
| 1 | A | 78 | LYS | Peptide |
| 1 | B | 107 | LEU | Peptide |
| 1 | B | 167 | ILE | Peptide |
| 1 | B | 169 | GLU | Peptide |
| 1 | B | 170 | GLN | Peptide |
| 1 | C | 107 | LEU | Peptide |
| 1 | D | 107 | LEU | Peptide |
| 1 | E | 166 | MET | Peptide |
| 1 | E | 167 | ILE | Peptide |
| 1 | E | 169 | GLU | 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 | A | 3327 | 0 | 3287 | 294 | 0 |
| 1 | B | 3290 | 0 | 3253 | 317 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | C | 3275 | 0 | 3242 | 319 | 0 |
| 1 | D | 3298 | 0 | 3264 | 293 | 0 |
| 1 | E | 3327 | 0 | 3287 | 288 | 0 |
| 2 | R | 900 | 0 | 496 | 82 | 0 |
| 3 | A | 3 | 0 | 0 | 0 | 0 |
| 3 | B | 4 | 0 | 0 | 0 | 0 |
| 3 | C | 2 | 0 | 0 | 0 | 0 |
| 3 | D | 3 | 0 | 0 | 0 | 0 |
| 3 | E | 3 | 0 | 0 | 0 | 0 |
| 3 | R | 5 | 0 | 0 | 0 | 0 |
| All | All | 17437 | 0 | 16829 | 1458 | 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 43.

All (1458) 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) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:163:GLN:O | 1:E:167:ILE:HB | 1.36 | 1.25 |
| 1:B:317:ARG:HD3 | 2:R:22:C:O2' | 1.41 | 1.18 |
| 1:E:177:GLU:HA | 1:E:181:ILE:HD11 | 1.31 | 1.12 |
| 1:C:317:ARG:NH2 | 2:R:14:C:H5' | 1.64 | 1.11 |
| 1:A:317:ARG:NH2 | 2:R:32:C:H5' | 1.64 | 1.11 |
| 1:D:177:GLU:HA | 1:D:181:ILE:HD11 | 1.32 | 1.10 |
| 1:C:177:GLU:HA | 1:C:181:ILE:HD11 | 1.33 | 1.09 |
| 1:B:317:ARG:NH2 | 2:R:23:C:H5' | 1.66 | 1.09 |
| 1:B:60:LYS:O | 1:B:61:SER:HB3 | 1.53 | 1.09 |
| 1:D:364:LEU:HD23 | 1:D:365:THR:H | 1.16 | 1.09 |
| 1:A:177:GLU:HA | 1:A:181:ILE:HD11 | 1.33 | 1.09 |
| 1:E:169:GLU:HG2 | 1:E:170:GLN:H | 1.15 | 1.06 |
| 1:B:168:ASN:O | 1:B:169:GLU:HG2 | 1.53 | 1.05 |
| 1:B:177:GLU:HA | 1:B:181:ILE:HD11 | 1.33 | 1.05 |
| 1:D:72:TYR:HE1 | 1:D:134:LEU:HD12 | 1.22 | 1.05 |
| 1:E:72:TYR:HE1 | 1:E:134:LEU:HD12 | 1.21 | 1.04 |
| 1:B:72:TYR:HE1 | 1:B:134:LEU:HD12 | 1.22 | 1.04 |
| 1:E:317:ARG:NH2 | 2:R:41:C:H5' | 1.72 | 1.02 |
| 1:D:263:LEU:HD12 | 1:D:264:PRO:HD2 | 1.42 | 1.02 |
| 1:E:263:LEU:HD12 | 1:E:264:PRO:HD2 | 1.41 | 1.01 |
| 1:A:263:LEU:HD12 | 1:A:264:PRO:HD2 | 1.40 | 1.01 |
| 1:B:263:LEU:HD12 | 1:B:264:PRO:HD2 | 1.45 | 0.98 |
| 1:C:263:LEU:HD12 | 1:C:264:PRO:HD2 | 1.46 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:117:LEU:HB2 | 1:B:118:PRO:HD3 | 1.44 | 0.97 |
| 1:A:72:TYR:HE1 | 1:A:134:LEU:HD12 | 1.28 | 0.97 |
| 1:A:165:LYS:O | 1:A:167:ILE:HD12 | 1.65 | 0.96 |
| 1:B:356:THR:HG23 | 1:B:357:PRO:HD3 | 1.46 | 0.96 |
| 1:C:356:THR:HG23 | 1:C:357:PRO:HD3 | 1.45 | 0.95 |
| 1:B:317:ARG:HD3 | 2:R:22:C:HO2' | 1.32 | 0.95 |
| 1:A:117:LEU:HB2 | 1:A:118:PRO:HD3 | 1.48 | 0.95 |
| 1:C:72:TYR:HE1 | 1:C:134:LEU:HD12 | 1.28 | 0.94 |
| 1:D:356:THR:HG23 | 1:D:357:PRO:HD3 | 1.50 | 0.94 |
| 1:A:60:LYS:O | 1:A:61:SER:HB3 | 1.68 | 0.93 |
| 1:A:356:THR:HG23 | 1:A:357:PRO:HD3 | 1.51 | 0.93 |
| 1:E:117:LEU:HB2 | 1:E:118:PRO:HD3 | 1.51 | 0.92 |
| 1:D:43:ASN:HA | 1:D:111:LYS:HG3 | 1.48 | 0.92 |
| 1:B:43:ASN:HA | 1:B:111:LYS:HG3 | 1.50 | 0.92 |
| 1:C:317:ARG:HD3 | 2:R:13:C:O2' | 1.68 | 0.91 |
| 1:A:65:SER:HB2 | 1:A:117:LEU:HD11 | 1.50 | 0.91 |
| 1:E:43:ASN:HA | 1:E:111:LYS:HG3 | 1.51 | 0.91 |
| 1:D:65:SER:HB2 | 1:D:117:LEU:HD11 | 1.51 | 0.91 |
| 1:E:356:THR:HG23 | 1:E:357:PRO:HD3 | 1.49 | 0.91 |
| 1:C:43:ASN:HA | 1:C:111:LYS:HG3 | 1.49 | 0.91 |
| 1:C:117:LEU:HB2 | 1:C:118:PRO:HD3 | 1.50 | 0.91 |
| 1:E:65:SER:HB2 | 1:E:117:LEU:HD11 | 1.50 | 0.90 |
| 1:E:60:LYS:O | 1:E:61:SER:HB3 | 1.72 | 0.90 |
| 1:B:150:PRO:HA | 1:B:152:TYR:CE1 | 2.05 | 0.90 |
| 1:B:380:GLY:HA2 | 1:C:354:LYS:HZ3 | 1.37 | 0.90 |
| 1:A:43:ASN:HA | 1:A:111:LYS:HG3 | 1.51 | 0.90 |
| 1:D:117:LEU:HB2 | 1:D:118:PRO:HD3 | 1.52 | 0.89 |
| 1:C:317:ARG:NE | 1:C:317:ARG:H | 1.70 | 0.89 |
| 1:B:164:CYS:HA | 1:B:168:ASN:HA | 1.52 | 0.89 |
| 1:D:354:LYS:HE3 | 1:D:356:THR:HA | 1.55 | 0.89 |
| 1:C:150:PRO:HA | 1:C:152:TYR:CE1 | 2.08 | 0.89 |
| 1:A:150:PRO:HA | 1:A:152:TYR:CE1 | 2.07 | 0.89 |
| 1:C:65:SER:HB2 | 1:C:117:LEU:HD11 | 1.51 | 0.89 |
| 1:E:354:LYS:HE3 | 1:E:356:THR:HA | 1.55 | 0.89 |
| 1:D:316:ALA:HA | 1:D:317:ARG:NH2 | 1.88 | 0.89 |
| 1:B:317:ARG:CD | 2:R:22:C:O2' | 2.20 | 0.88 |
| 1:B:380:GLY:HA2 | 1:C:354:LYS:NZ | 1.88 | 0.88 |
| 1:B:65:SER:HB2 | 1:B:117:LEU:HD11 | 1.52 | 0.88 |
| 1:E:317:ARG:HG3 | 2:R:40:C:N3 | 1.88 | 0.87 |
| 1:C:167:ILE:O | 1:C:169:GLU:HG2 | 1.74 | 0.87 |
| 1:B:177:GLU:HG2 | 1:B:179:ARG:H | 1.40 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:42:ILE:HD12 | 1:D:74:TYR:HB2 | 1.55 | 0.87 |
| 1:A:42:ILE:HD12 | 1:A:74:TYR:HB2 | 1.57 | 0.86 |
| 1:D:150:PRO:HA | 1:D:152:TYR:CE1 | 2.11 | 0.86 |
| 1:C:177:GLU:HG2 | 1:C:179:ARG:H | 1.40 | 0.85 |
| 1:C:354:LYS:HE3 | 1:C:356:THR:HA | 1.57 | 0.85 |
| 1:D:60:LYS:O | 1:D:61:SER:HB3 | 1.73 | 0.85 |
| 1:E:169:GLU:HG2 | 1:E:170:GLN:N | 1.86 | 0.85 |
| 1:A:177:GLU:HG2 | 1:A:179:ARG:H | 1.41 | 0.84 |
| 1:B:168:ASN:C | 1:B:169:GLU:HG2 | 1.93 | 0.84 |
| 1:E:165:LYS:O | 1:E:167:ILE:HG13 | 1.76 | 0.84 |
| 1:B:354:LYS:HE3 | 1:B:356:THR:HA | 1.59 | 0.84 |
| 1:C:376:VAL:HG13 | 1:D:354:LYS:HB2 | 1.57 | 0.84 |
| 1:B:42:ILE:HD12 | 1:B:74:TYR:HB2 | 1.57 | 0.84 |
| 1:D:72:TYR:CE1 | 1:D:134:LEU:HD12 | 2.12 | 0.84 |
| 1:E:150:PRO:HA | 1:E:152:TYR:CE1 | 2.11 | 0.84 |
| 1:D:165:LYS:O | 1:D:167:ILE:HD12 | 1.78 | 0.84 |
| 1:E:163:GLN:O | 1:E:167:ILE:CB | 2.22 | 0.84 |
| 1:C:165:LYS:HG2 | 1:C:166:MET:HG3 | 1.58 | 0.84 |
| 1:D:177:GLU:HG2 | 1:D:179:ARG:H | 1.43 | 0.84 |
| 1:C:317:ARG:HH21 | 2:R:14:C:H5' | 1.40 | 0.83 |
| 1:E:42:ILE:HD12 | 1:E:74:TYR:HB2 | 1.57 | 0.83 |
| 1:E:177:GLU:HG2 | 1:E:179:ARG:H | 1.41 | 0.83 |
| 1:D:74:TYR:CE1 | 1:D:78:LYS:HD2 | 2.14 | 0.83 |
| 1:E:72:TYR:CE1 | 1:E:134:LEU:HD12 | 2.11 | 0.82 |
| 1:D:317:ARG:H | 1:D:317:ARG:NE | 1.77 | 0.82 |
| 1:E:37:GLU:HB2 | 1:E:108:VAL:HG11 | 1.61 | 0.82 |
| 1:B:317:ARG:NE | 1:B:317:ARG:H | 1.76 | 0.82 |
| 1:A:354:LYS:HE3 | 1:A:356:THR:HA | 1.62 | 0.81 |
| 1:B:376:VAL:HG21 | 1:C:352:ASP:OD1 | 1.80 | 0.81 |
| 1:B:317:ARG:HH21 | 2:R:23:C:H5' | 1.43 | 0.81 |
| 1:C:60:LYS:O | 1:C:61:SER:HB3 | 1.78 | 0.81 |
| 1:B:2:SER:O | 1:C:243:GLU:HG3 | 1.81 | 0.81 |
| 1:A:376:VAL:HG21 | 1:B:352:ASP:OD1 | 1.82 | 0.80 |
| 1:C:317:ARG:CD | 2:R:13:C:O2' | 2.29 | 0.80 |
| 1:A:316:ALA:HA | 1:A:317:ARG:NH2 | 1.97 | 0.80 |
| 1:C:42:ILE:HD12 | 1:C:74:TYR:HB2 | 1.63 | 0.80 |
| 1:E:74:TYR:CE1 | 1:E:78:LYS:HD2 | 2.17 | 0.79 |
| 1:D:37:GLU:HB2 | 1:D:108:VAL:HG11 | 1.63 | 0.79 |
| 1:C:72:TYR:CE1 | 1:C:134:LEU:HD12 | 2.17 | 0.79 |
| 1:A:37:GLU:HB2 | 1:A:108:VAL:HG11 | 1.64 | 0.79 |
| 1:A:166:MET:H | 1:E:184:VAL:HG11 | 1.47 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:74:TYR:CE1 | 1:B:78:LYS:HD2 | 2.18 | 0.78 |
| 1:E:136:LEU:HD22 | 1:E:163:GLN:HE21 | 1.48 | 0.78 |
| 1:E:169:GLU:CG | 1:E:170:GLN:H | 1.95 | 0.78 |
| 1:D:364:LEU:HD23 | 1:D:365:THR:N | 1.98 | 0.78 |
| 1:B:72:TYR:CE1 | 1:B:134:LEU:HD12 | 2.12 | 0.78 |
| 1:C:37:GLU:HB2 | 1:C:108:VAL:HG11 | 1.64 | 0.78 |
| 1:A:126:ARG:HA | 1:A:126:ARG:HH11 | 1.48 | 0.78 |
| 1:A:317:ARG:NE | 1:A:317:ARG:H | 1.80 | 0.78 |
| 1:C:136:LEU:HD22 | 1:C:163:GLN:HE21 | 1.47 | 0.78 |
| 1:B:54:TYR:CE1 | 1:B:118:PRO:HB2 | 2.19 | 0.78 |
| 1:A:74:TYR:CE1 | 1:A:78:LYS:HD2 | 2.19 | 0.78 |
| 1:D:214:ARG:HA | 1:D:217:THR:HG22 | 1.65 | 0.78 |
| 1:A:389:PRO:HA | 1:A:393:MET:HE1 | 1.66 | 0.78 |
| 1:B:133:TRP:HB3 | 1:B:167:ILE:HD13 | 1.64 | 0.77 |
| 1:E:126:ARG:HA | 1:E:126:ARG:HH11 | 1.49 | 0.77 |
| 1:B:316:ALA:HA | 1:B:317:ARG:NH2 | 1.99 | 0.77 |
| 1:B:47:SER:HB3 | 1:B:50:ASP:HB2 | 1.67 | 0.77 |
| 1:D:44:THR:HG22 | 1:D:46:LYS:HG2 | 1.67 | 0.77 |
| 2:R:21:C:H6 | 2:R:21:C:H5'' | 1.49 | 0.77 |
| 1:B:214:ARG:HA | 1:B:217:THR:HG22 | 1.67 | 0.76 |
| 1:B:44:THR:HG22 | 1:B:46:LYS:HG2 | 1.68 | 0.76 |
| 1:C:74:TYR:CE1 | 1:C:78:LYS:HD2 | 2.20 | 0.76 |
| 1:B:349:CYS:SG | 1:E:8:ILE:HG22 | 2.25 | 0.76 |
| 1:E:54:TYR:CE1 | 1:E:118:PRO:HB2 | 2.21 | 0.76 |
| 1:C:165:LYS:NZ | 1:C:165:LYS:HB2 | 2.00 | 0.76 |
| 1:A:44:THR:HG23 | 1:A:46:LYS:HE2 | 1.68 | 0.75 |
| 1:D:317:ARG:H | 1:D:317:ARG:CZ | 1.98 | 0.75 |
| 1:A:317:ARG:HH21 | 2:R:32:C:H5' | 1.48 | 0.75 |
| 1:D:54:TYR:CE1 | 1:D:118:PRO:HB2 | 2.21 | 0.75 |
| 1:E:389:PRO:HA | 1:E:393:MET:HE1 | 1.68 | 0.75 |
| 1:A:214:ARG:HA | 1:A:217:THR:HG22 | 1.68 | 0.75 |
| 1:E:214:ARG:HA | 1:E:217:THR:HG22 | 1.68 | 0.75 |
| 1:A:54:TYR:CE1 | 1:A:118:PRO:HB2 | 2.22 | 0.75 |
| 1:B:37:GLU:HB2 | 1:B:108:VAL:HG11 | 1.67 | 0.75 |
| 1:A:47:SER:HB3 | 1:A:50:ASP:HB2 | 1.69 | 0.75 |
| 1:D:136:LEU:HD22 | 1:D:163:GLN:HE21 | 1.50 | 0.74 |
| 1:C:184:VAL:HG13 | 1:D:165:LYS:HG3 | 1.69 | 0.74 |
| 1:A:72:TYR:CE1 | 1:A:134:LEU:HD12 | 2.18 | 0.74 |
| 1:A:136:LEU:HD22 | 1:A:163:GLN:HE21 | 1.52 | 0.74 |
| 2:R:18:C:H2' | 2:R:19:C:O4' | 1.87 | 0.74 |
| 1:A:226:ALA:HB2 | 2:R:31:C:H5' | 1.69 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:214:ARG:HA | 1:C:217:THR:HG22 | 1.69 | 0.74 |
| 1:A:60:LYS:O | 1:A:61:SER:CB | 2.36 | 0.74 |
| 1:A:380:GLY:HA2 | 1:B:354:LYS:HZ3 | 1.52 | 0.74 |
| 1:C:44:THR:HG22 | 1:C:46:LYS:HG2 | 1.69 | 0.74 |
| 1:B:136:LEU:HD22 | 1:B:163:GLN:HE21 | 1.52 | 0.74 |
| 1:B:230:THR:HG21 | 1:B:298:HIS:CE1 | 2.23 | 0.73 |
| 1:D:151:GLU:OE1 | 1:D:155:LYS:NZ | 2.21 | 0.73 |
| 1:B:383:GLU:HG3 | 1:C:354:LYS:HE2 | 1.71 | 0.73 |
| 1:D:126:ARG:HH11 | 1:D:126:ARG:HA | 1.52 | 0.73 |
| 1:E:133:TRP:HB3 | 1:E:167:ILE:HD13 | 1.69 | 0.73 |
| 1:C:181:ILE:HD12 | 1:C:181:ILE:H | 1.52 | 0.73 |
| 1:B:376:VAL:HG13 | 1:C:354:LYS:HB2 | 1.71 | 0.73 |
| 1:D:91:PHE:CZ | 1:D:267:GLU:HG3 | 2.24 | 0.73 |
| 1:A:2:SER:O | 1:B:243:GLU:HG3 | 1.88 | 0.73 |
| 1:B:171:PHE:CZ | 1:B:173:PRO:HG2 | 2.24 | 0.73 |
| 1:D:364:LEU:HD22 | 1:D:368:ALA:HB2 | 1.70 | 0.73 |
| 1:A:167:ILE:HG22 | 1:A:169:GLU:HG2 | 1.71 | 0.73 |
| 1:B:126:ARG:HH11 | 1:B:126:ARG:HA | 1.52 | 0.73 |
| 1:A:380:GLY:HA2 | 1:B:354:LYS:NZ | 2.04 | 0.73 |
| 1:C:380:GLY:HA2 | 1:D:354:LYS:NZ | 2.04 | 0.72 |
| 1:D:230:THR:HG21 | 1:D:298:HIS:CE1 | 2.24 | 0.72 |
| 1:D:27:TYR:HB3 | 1:D:266:GLN:NE2 | 2.04 | 0.72 |
| 1:E:317:ARG:H | 1:E:317:ARG:NE | 1.87 | 0.72 |
| 1:E:364:LEU:HB2 | 1:E:368:ALA:HB2 | 1.70 | 0.72 |
| 1:C:317:ARG:O | 1:C:319:PRO:HD3 | 1.90 | 0.72 |
| 1:D:74:TYR:CD1 | 1:D:78:LYS:HD2 | 2.24 | 0.72 |
| 1:A:153:ARG:HH12 | 1:A:176:PRO:C | 1.92 | 0.72 |
| 2:R:36:C:H2' | 2:R:37:C:O4' | 1.90 | 0.72 |
| 1:E:288:PRO:HG2 | 1:E:289:TYR:CE2 | 2.24 | 0.72 |
| 1:E:47:SER:HB3 | 1:E:50:ASP:HB2 | 1.71 | 0.72 |
| 1:B:44:THR:HG23 | 1:B:46:LYS:HE2 | 1.71 | 0.72 |
| 1:E:44:THR:HG23 | 1:E:46:LYS:HE2 | 1.72 | 0.72 |
| 1:E:60:LYS:O | 1:E:61:SER:CB | 2.37 | 0.72 |
| 1:D:42:ILE:CD1 | 1:D:74:TYR:HB2 | 2.18 | 0.72 |
| 1:D:29:ALA:HB2 | 1:D:91:PHE:CE2 | 2.25 | 0.72 |
| 1:C:126:ARG:HH11 | 1:C:126:ARG:HA | 1.52 | 0.72 |
| 1:B:60:LYS:O | 1:B:61:SER:CB | 2.33 | 0.72 |
| 1:E:316:ALA:HA | 1:E:317:ARG:NH2 | 2.04 | 0.72 |
| 1:B:29:ALA:HB2 | 1:B:91:PHE:HE2 | 1.54 | 0.72 |
| 1:B:184:VAL:HG11 | 1:C:166:MET:H | 1.55 | 0.72 |
| 1:D:44:THR:HG23 | 1:D:46:LYS:HE2 | 1.72 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:44:THR:HG23 | 1:C:46:LYS:HE2 | 1.72 | 0.72 |
| 1:E:74:TYR:CD1 | 1:E:78:LYS:HD2 | 2.25 | 0.72 |
| 1:D:29:ALA:HB2 | 1:D:91:PHE:HE2 | 1.54 | 0.72 |
| 1:A:181:ILE:H | 1:A:181:ILE:HD12 | 1.54 | 0.71 |
| 1:A:42:ILE:CD1 | 1:A:74:TYR:HB2 | 2.21 | 0.71 |
| 1:C:54:TYR:CE1 | 1:C:118:PRO:HB2 | 2.25 | 0.71 |
| 1:A:74:TYR:CD1 | 1:A:78:LYS:HD2 | 2.26 | 0.71 |
| 1:D:41:TYR:HE1 | 1:D:110:LEU:HD12 | 1.56 | 0.71 |
| 1:E:130:ASP:C | 1:E:132:LYS:H | 1.93 | 0.71 |
| 1:C:389:PRO:HA | 1:C:393:MET:HE2 | 1.72 | 0.71 |
| 1:C:230:THR:HG21 | 1:C:298:HIS:CE1 | 2.26 | 0.71 |
| 1:D:47:SER:HB3 | 1:D:50:ASP:HB2 | 1.73 | 0.71 |
| 1:B:317:ARG:O | 1:B:319:PRO:HD3 | 1.91 | 0.71 |
| 1:A:130:ASP:C | 1:A:132:LYS:H | 1.94 | 0.71 |
| 1:E:165:LYS:O | 1:E:167:ILE:CG1 | 2.39 | 0.70 |
| 1:C:316:ALA:HA | 1:C:317:ARG:NH2 | 2.06 | 0.70 |
| 1:A:44:THR:HG22 | 1:A:46:LYS:HG2 | 1.72 | 0.70 |
| 1:A:105:PHE:C | 1:A:107:LEU:H | 1.95 | 0.70 |
| 1:D:288:PRO:HG2 | 1:D:289:TYR:CE2 | 2.26 | 0.70 |
| 1:B:168:ASN:O | 1:B:169:GLU:CG | 2.36 | 0.70 |
| 1:C:47:SER:HB3 | 1:C:50:ASP:HB2 | 1.73 | 0.70 |
| 1:B:74:TYR:CD1 | 1:B:78:LYS:HD2 | 2.25 | 0.70 |
| 1:B:42:ILE:CD1 | 1:B:74:TYR:HB2 | 2.21 | 0.70 |
| 1:D:130:ASP:C | 1:D:132:LYS:H | 1.93 | 0.70 |
| 1:C:317:ARG:NE | 2:R:13:C:O2' | 2.24 | 0.70 |
| 1:A:354:LYS:HB2 | 1:E:376:VAL:HG13 | 1.73 | 0.70 |
| 1:A:168:ASN:O | 1:A:169:GLU:OE2 | 2.09 | 0.70 |
| 1:E:44:THR:HG22 | 1:E:46:LYS:HG2 | 1.72 | 0.70 |
| 1:E:91:PHE:CZ | 1:E:267:GLU:HG3 | 2.26 | 0.70 |
| 1:D:317:ARG:NH2 | 2:R:5:C:O5' | 2.25 | 0.70 |
| 1:E:230:THR:HG21 | 1:E:298:HIS:CE1 | 2.26 | 0.70 |
| 1:D:389:PRO:HA | 1:D:393:MET:HE2 | 1.73 | 0.70 |
| 1:E:45:THR:H | 1:E:111:LYS:HZ1 | 1.38 | 0.70 |
| 1:B:398:LYS:HG2 | 1:B:402:MET:HE2 | 1.73 | 0.69 |
| 1:A:376:VAL:HG13 | 1:B:354:LYS:HB2 | 1.74 | 0.69 |
| 1:C:380:GLY:HA2 | 1:D:354:LYS:HZ3 | 1.56 | 0.69 |
| 1:A:317:ARG:O | 1:A:319:PRO:HD3 | 1.92 | 0.69 |
| 1:E:42:ILE:CD1 | 1:E:74:TYR:HB2 | 2.22 | 0.69 |
| 1:B:171:PHE:CG | 1:B:172:GLU:N | 2.60 | 0.69 |
| 1:C:149:MET:O | 1:C:151:GLU:N | 2.26 | 0.69 |
| 1:C:74:TYR:CD1 | 1:C:78:LYS:HD2 | 2.27 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:199:ASP:OD1 | 1:D:214:ARG:HD2 | 1.93 | 0.69 |
| 1:B:117:LEU:HB2 | 1:B:118:PRO:CD | 2.22 | 0.69 |
| 1:A:167:ILE:HG22 | 1:A:169:GLU:CG | 2.23 | 0.69 |
| 1:C:376:VAL:HG21 | 1:D:352:ASP:OD1 | 1.92 | 0.69 |
| 1:B:253:GLU:H | 1:B:253:GLU:CD | 1.96 | 0.69 |
| 1:B:130:ASP:C | 1:B:132:LYS:H | 1.95 | 0.69 |
| 1:E:153:ARG:HH12 | 1:E:176:PRO:C | 1.96 | 0.69 |
| 1:A:44:THR:CG2 | 1:A:46:LYS:HE2 | 2.23 | 0.69 |
| 1:C:130:ASP:C | 1:C:132:LYS:H | 1.95 | 0.69 |
| 1:C:29:ALA:HB2 | 1:C:91:PHE:HE2 | 1.57 | 0.69 |
| 1:A:91:PHE:CZ | 1:A:267:GLU:HG3 | 2.27 | 0.69 |
| 1:D:253:GLU:CD | 1:D:253:GLU:H | 1.96 | 0.69 |
| 1:E:164:CYS:O | 1:E:168:ASN:OD1 | 2.11 | 0.69 |
| 1:B:105:PHE:C | 1:B:107:LEU:H | 1.96 | 0.69 |
| 1:D:149:MET:O | 1:D:151:GLU:N | 2.26 | 0.68 |
| 1:B:173:PRO:C | 1:B:174:LEU:HG | 2.12 | 0.68 |
| 1:C:398:LYS:HG2 | 1:C:402:MET:HE3 | 1.74 | 0.68 |
| 1:A:230:THR:HG21 | 1:A:298:HIS:CE1 | 2.28 | 0.68 |
| 1:A:165:LYS:HB2 | 1:A:165:LYS:NZ | 2.08 | 0.68 |
| 1:B:29:ALA:HB2 | 1:B:91:PHE:CE2 | 2.28 | 0.68 |
| 2:R:7:C:OP2 | 2:R:7:C:H4' | 1.94 | 0.68 |
| 1:B:18:LEU:CD1 | 1:C:232:GLY:HA2 | 2.24 | 0.68 |
| 1:E:253:GLU:CD | 1:E:253:GLU:H | 1.97 | 0.68 |
| 1:B:97:LYS:O | 1:B:100:ASP:HB2 | 1.92 | 0.68 |
| 1:B:181:ILE:H | 1:B:181:ILE:HD12 | 1.59 | 0.68 |
| 1:D:173:PRO:C | 1:D:174:LEU:HG | 2.12 | 0.68 |
| 1:C:288:PRO:HG2 | 1:C:289:TYR:CE2 | 2.28 | 0.68 |
| 1:B:27:TYR:HB3 | 1:B:266:GLN:NE2 | 2.09 | 0.68 |
| 1:D:45:THR:H | 1:D:111:LYS:HZ1 | 1.40 | 0.67 |
| 1:B:262:MET:HE2 | 1:B:262:MET:HA | 1.75 | 0.67 |
| 1:A:67:ILE:H | 1:A:67:ILE:HD12 | 1.59 | 0.67 |
| 1:B:91:PHE:CZ | 1:B:267:GLU:HG3 | 2.28 | 0.67 |
| 1:C:317:ARG:CZ | 1:C:317:ARG:H | 2.06 | 0.67 |
| 1:E:181:ILE:H | 1:E:181:ILE:HD12 | 1.60 | 0.67 |
| 1:E:317:ARG:O | 1:E:319:PRO:HD3 | 1.95 | 0.67 |
| 1:E:25:VAL:HG11 | 1:E:288:PRO:HA | 1.77 | 0.67 |
| 1:B:45:THR:H | 1:B:111:LYS:HZ1 | 1.42 | 0.67 |
| 1:C:29:ALA:HB2 | 1:C:91:PHE:CE2 | 2.30 | 0.67 |
| 1:C:148:GLN:HG2 | 1:C:179:ARG:NH1 | 2.09 | 0.67 |
| 1:A:153:ARG:NH1 | 1:A:176:PRO:C | 2.48 | 0.67 |
| 1:C:105:PHE:C | 1:C:107:LEU:H | 1.98 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:153:ARG:HH12 | 1:D:176:PRO:C | 1.98 | 0.67 |
| 1:E:149:MET:O | 1:E:151:GLU:N | 2.28 | 0.67 |
| 1:D:317:ARG:CZ | 2:R:5:C:OP2 | 2.43 | 0.67 |
| 1:E:67:ILE:H | 1:E:67:ILE:HD12 | 1.60 | 0.67 |
| 1:E:41:TYR:HE1 | 1:E:110:LEU:HD12 | 1.59 | 0.67 |
| 1:A:97:LYS:O | 1:A:100:ASP:HB2 | 1.95 | 0.67 |
| 1:E:105:PHE:C | 1:E:107:LEU:H | 1.98 | 0.66 |
| 1:A:199:ASP:OD1 | 1:A:214:ARG:HD2 | 1.95 | 0.66 |
| 1:A:7:ARG:NH1 | 1:B:259:VAL:HG21 | 2.09 | 0.66 |
| 1:D:262:MET:HA | 1:D:262:MET:HE2 | 1.75 | 0.66 |
| 1:C:2:SER:O | 1:D:243:GLU:HG3 | 1.95 | 0.66 |
| 1:E:173:PRO:C | 1:E:174:LEU:HG | 2.14 | 0.66 |
| 1:B:117:LEU:CB | 1:B:118:PRO:HD3 | 2.23 | 0.66 |
| 1:A:165:LYS:O | 1:A:166:MET:HB2 | 1.95 | 0.66 |
| 1:C:42:ILE:CD1 | 1:C:74:TYR:HB2 | 2.24 | 0.66 |
| 1:C:167:ILE:O | 1:C:169:GLU:CG | 2.42 | 0.66 |
| 1:A:151:GLU:OE1 | 1:A:155:LYS:NZ | 2.29 | 0.66 |
| 1:B:107:LEU:HD12 | 1:B:107:LEU:N | 2.10 | 0.66 |
| 1:B:199:ASP:OD1 | 1:B:214:ARG:HD2 | 1.95 | 0.66 |
| 1:E:226:ALA:O | 1:E:230:THR:HG23 | 1.96 | 0.66 |
| 1:C:173:PRO:C | 1:C:174:LEU:HG | 2.15 | 0.66 |
| 1:C:149:MET:C | 1:C:151:GLU:H | 1.99 | 0.66 |
| 1:A:253:GLU:CD | 1:A:253:GLU:H | 1.99 | 0.66 |
| 1:D:81:ARG:CB | 1:D:208:HIS:HE2 | 2.09 | 0.66 |
| 1:C:27:TYR:HB3 | 1:C:266:GLN:NE2 | 2.10 | 0.66 |
| 1:E:164:CYS:HA | 1:E:168:ASN:HA | 1.77 | 0.66 |
| 1:E:302:GLN:HG2 | 1:E:316:ALA:CB | 2.26 | 0.66 |
| 1:A:27:TYR:HB3 | 1:A:266:GLN:NE2 | 2.11 | 0.65 |
| 1:E:199:ASP:OD1 | 1:E:214:ARG:HD2 | 1.96 | 0.65 |
| 1:B:18:LEU:HD12 | 1:C:232:GLY:HA2 | 1.78 | 0.65 |
| 1:A:302:GLN:HG2 | 1:A:316:ALA:CB | 2.27 | 0.65 |
| 1:C:151:GLU:OE1 | 1:C:155:LYS:NZ | 2.29 | 0.65 |
| 1:B:149:MET:O | 1:B:151:GLU:N | 2.30 | 0.65 |
| 1:C:376:VAL:HG13 | 1:D:354:LYS:CB | 2.26 | 0.65 |
| 1:B:106:ASP:C | 1:B:107:LEU:HD12 | 2.16 | 0.65 |
| 1:B:317:ARG:NE | 1:B:317:ARG:N | 2.44 | 0.65 |
| 1:C:317:ARG:NE | 2:R:13:C:HO2' | 1.95 | 0.65 |
| 1:D:181:ILE:H | 1:D:181:ILE:HD12 | 1.62 | 0.65 |
| 1:B:148:GLN:HG2 | 1:B:179:ARG:NH1 | 2.11 | 0.65 |
| 1:B:151:GLU:OE1 | 1:B:155:LYS:NZ | 2.29 | 0.65 |
| 1:D:149:MET:C | 1:D:151:GLU:H | 2.00 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:117:LEU:HB2 | 1:A:118:PRO:CD | 2.25 | 0.65 |
| 1:A:173:PRO:C | 1:A:174:LEU:HG | 2.16 | 0.65 |
| 1:E:357:PRO:HA | 1:E:360:SER:OG | 1.96 | 0.65 |
| 1:C:61:SER:O | 1:C:63:ASN:N | 2.30 | 0.65 |
| 1:D:97:LYS:O | 1:D:100:ASP:HB2 | 1.97 | 0.65 |
| 1:A:226:ALA:HB2 | 2:R:31:C:C5' | 2.26 | 0.65 |
| 1:B:67:ILE:HD12 | 1:B:67:ILE:H | 1.62 | 0.65 |
| 1:C:41:TYR:HE1 | 1:C:110:LEU:HD12 | 1.61 | 0.65 |
| 1:B:317:ARG:CZ | 1:B:317:ARG:H | 2.10 | 0.64 |
| 1:D:61:SER:O | 1:D:63:ASN:N | 2.30 | 0.64 |
| 1:D:143:ARG:HH12 | 2:R:9:C:H5' | 1.63 | 0.64 |
| 1:E:44:THR:CG2 | 1:E:46:LYS:HE2 | 2.28 | 0.64 |
| 1:D:226:ALA:O | 1:D:230:THR:HG23 | 1.98 | 0.64 |
| 1:E:81:ARG:CB | 1:E:208:HIS:HE2 | 2.11 | 0.64 |
| 1:C:153:ARG:HH12 | 1:C:176:PRO:C | 2.00 | 0.64 |
| 1:A:263:LEU:CD1 | 1:A:264:PRO:HD2 | 2.23 | 0.64 |
| 1:A:29:ALA:HB2 | 1:A:91:PHE:HE2 | 1.62 | 0.64 |
| 1:D:67:ILE:HD12 | 1:D:67:ILE:H | 1.61 | 0.64 |
| 1:B:81:ARG:CB | 1:B:208:HIS:HE2 | 2.11 | 0.64 |
| 1:B:153:ARG:HH12 | 1:B:176:PRO:C | 2.01 | 0.64 |
| 1:C:253:GLU:H | 1:C:253:GLU:CD | 2.01 | 0.64 |
| 1:A:41:TYR:HE1 | 1:A:110:LEU:HD12 | 1.62 | 0.64 |
| 1:E:262:MET:HA | 1:E:262:MET:HE2 | 1.77 | 0.64 |
| 1:C:67:ILE:H | 1:C:67:ILE:HD12 | 1.63 | 0.64 |
| 1:D:364:LEU:CD2 | 1:D:365:THR:H | 2.04 | 0.64 |
| 1:C:117:LEU:HB2 | 1:C:118:PRO:CD | 2.27 | 0.64 |
| 1:D:44:THR:CG2 | 1:D:46:LYS:HE2 | 2.27 | 0.64 |
| 1:E:214:ARG:HA | 1:E:217:THR:CG2 | 2.28 | 0.64 |
| 1:B:389:PRO:HA | 1:B:393:MET:HE1 | 1.80 | 0.64 |
| 1:B:44:THR:CG2 | 1:B:46:LYS:HE2 | 2.27 | 0.64 |
| 1:D:50:ASP:OD2 | 1:D:120:GLY:HA2 | 1.98 | 0.64 |
| 1:B:165:LYS:O | 1:B:167:ILE:HD12 | 1.98 | 0.64 |
| 1:D:155:LYS:NZ | 2:R:8:C:OP2 | 2.28 | 0.64 |
| 1:E:97:LYS:O | 1:E:100:ASP:HB2 | 1.98 | 0.64 |
| 1:B:288:PRO:HG2 | 1:B:289:TYR:CE2 | 2.32 | 0.64 |
| 1:E:153:ARG:NH1 | 1:E:176:PRO:C | 2.52 | 0.63 |
| 1:C:97:LYS:O | 1:C:100:ASP:HB2 | 1.97 | 0.63 |
| 1:E:148:GLN:HG2 | 1:E:179:ARG:NH1 | 2.13 | 0.63 |
| 1:A:317:ARG:CZ | 1:A:317:ARG:H | 2.11 | 0.63 |
| 1:D:317:ARG:NH1 | 2:R:5:C:OP2 | 2.32 | 0.63 |
| 1:C:228:LEU:HB2 | 1:C:289:TYR:HB3 | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:43:ASN:O | 1:A:44:THR:C | 2.36 | 0.63 |
| 1:C:165:LYS:O | 1:C:166:MET:HB2 | 1.97 | 0.63 |
| 1:E:375:VAL:O | 1:E:379:LEU:HB2 | 1.99 | 0.63 |
| 1:D:148:GLN:HG2 | 1:D:179:ARG:NH1 | 2.13 | 0.63 |
| 1:A:383:GLU:HG3 | 1:B:354:LYS:HE2 | 1.80 | 0.63 |
| 1:D:117:LEU:CB | 1:D:118:PRO:HD3 | 2.27 | 0.63 |
| 1:B:184:VAL:HG11 | 1:C:166:MET:N | 2.13 | 0.63 |
| 1:A:288:PRO:HG2 | 1:A:289:TYR:CE2 | 2.34 | 0.63 |
| 1:D:148:GLN:O | 1:D:152:TYR:HE2 | 1.82 | 0.63 |
| 1:C:117:LEU:CB | 1:C:118:PRO:HD3 | 2.27 | 0.63 |
| 1:C:81:ARG:CB | 1:C:208:HIS:HE2 | 2.11 | 0.63 |
| 1:B:50:ASP:OD2 | 1:B:120:GLY:HA2 | 1.98 | 0.63 |
| 1:D:31:TYR:CD1 | 1:D:31:TYR:C | 2.71 | 0.63 |
| 1:B:18:LEU:HD12 | 1:C:232:GLY:CA | 2.29 | 0.63 |
| 1:A:317:ARG:HD3 | 2:R:31:C:H2' | 1.80 | 0.63 |
| 1:D:29:ALA:O | 1:D:31:TYR:N | 2.30 | 0.63 |
| 1:B:89:SER:O | 1:B:90:SER:HB2 | 1.99 | 0.63 |
| 1:E:43:ASN:O | 1:E:44:THR:C | 2.37 | 0.63 |
| 1:B:31:TYR:C | 1:B:31:TYR:CD1 | 2.71 | 0.63 |
| 1:D:105:PHE:C | 1:D:107:LEU:H | 2.02 | 0.63 |
| 1:B:168:ASN:C | 1:B:169:GLU:CG | 2.65 | 0.62 |
| 1:C:44:THR:CG2 | 1:C:46:LYS:HE2 | 2.28 | 0.62 |
| 1:C:59:LEU:O | 1:C:61:SER:N | 2.29 | 0.62 |
| 1:E:149:MET:C | 1:E:151:GLU:H | 2.01 | 0.62 |
| 1:E:410:LYS:NZ | 2:R:40:C:H42 | 1.98 | 0.62 |
| 1:D:214:ARG:HA | 1:D:217:THR:CG2 | 2.29 | 0.62 |
| 1:C:302:GLN:HG2 | 1:C:316:ALA:CB | 2.30 | 0.62 |
| 1:C:42:ILE:HD12 | 1:C:74:TYR:HD2 | 1.62 | 0.62 |
| 1:A:89:SER:O | 1:A:90:SER:HB2 | 1.99 | 0.62 |
| 1:B:149:MET:C | 1:B:151:GLU:H | 2.02 | 0.62 |
| 1:B:380:GLY:CA | 1:C:354:LYS:HZ3 | 2.12 | 0.62 |
| 1:B:43:ASN:O | 1:B:44:THR:C | 2.38 | 0.62 |
| 1:B:25:VAL:HG11 | 1:B:288:PRO:HA | 1.82 | 0.62 |
| 1:A:127:THR:HG23 | 1:A:129:ALA:H | 1.64 | 0.62 |
| 1:B:375:VAL:O | 1:B:379:LEU:HB2 | 1.97 | 0.62 |
| 1:C:31:TYR:C | 1:C:31:TYR:CD1 | 2.72 | 0.62 |
| 1:A:228:LEU:HB2 | 1:A:289:TYR:HB3 | 1.82 | 0.62 |
| 1:E:133:TRP:CB | 1:E:167:ILE:HD13 | 2.29 | 0.62 |
| 1:A:117:LEU:CB | 1:A:118:PRO:HD3 | 2.26 | 0.62 |
| 1:D:127:THR:HG23 | 1:D:129:ALA:H | 1.64 | 0.62 |
| 1:D:153:ARG:NH1 | 1:D:176:PRO:C | 2.54 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:352:ASP:C | 1:B:352:ASP:OD1 | 2.38 | 0.62 |
| 1:D:302:GLN:HG2 | 1:D:316:ALA:CB | 2.30 | 0.62 |
| 1:C:91:PHE:CZ | 1:C:267:GLU:HG3 | 2.34 | 0.62 |
| 1:E:27:TYR:HB3 | 1:E:266:GLN:NE2 | 2.14 | 0.62 |
| 1:B:263:LEU:CD1 | 1:B:264:PRO:HD2 | 2.27 | 0.62 |
| 1:E:117:LEU:HB2 | 1:E:118:PRO:CD | 2.27 | 0.62 |
| 1:D:263:LEU:CD1 | 1:D:264:PRO:HD2 | 2.25 | 0.61 |
| 1:B:150:PRO:CA | 1:B:152:TYR:CE1 | 2.79 | 0.61 |
| 1:E:317:ARG:NH2 | 2:R:41:C:C5' | 2.58 | 0.61 |
| 1:A:375:VAL:O | 1:A:379:LEU:HB2 | 2.00 | 0.61 |
| 1:D:375:VAL:O | 1:D:379:LEU:HB2 | 2.00 | 0.61 |
| 1:A:226:ALA:O | 1:A:230:THR:HG23 | 2.00 | 0.61 |
| 1:C:45:THR:H | 1:C:111:LYS:HZ1 | 1.46 | 0.61 |
| 1:B:184:VAL:HG13 | 1:C:165:LYS:HG3 | 1.82 | 0.61 |
| 1:C:165:LYS:HZ2 | 1:C:165:LYS:HB2 | 1.64 | 0.61 |
| 1:C:199:ASP:OD1 | 1:C:214:ARG:HD2 | 1.99 | 0.61 |
| 1:E:89:SER:O | 1:E:90:SER:HB2 | 2.00 | 0.61 |
| 1:B:224:ASP:CG | 2:R:21:C:H4' | 2.20 | 0.61 |
| 1:A:107:LEU:HD12 | 1:A:107:LEU:N | 2.15 | 0.61 |
| 1:E:398:LYS:HG2 | 1:E:402:MET:HE3 | 1.83 | 0.61 |
| 1:C:29:ALA:O | 1:C:31:TYR:N | 2.30 | 0.61 |
| 1:C:323:GLU:OE1 | 1:D:239:GLY:HA3 | 2.01 | 0.61 |
| 1:A:317:ARG:HH22 | 2:R:32:C:H5' | 1.61 | 0.61 |
| 1:C:352:ASP:C | 1:C:352:ASP:OD1 | 2.38 | 0.61 |
| 1:D:117:LEU:HB2 | 1:D:118:PRO:CD | 2.28 | 0.61 |
| 1:D:228:LEU:HB2 | 1:D:289:TYR:HB3 | 1.80 | 0.61 |
| 1:A:149:MET:C | 1:A:151:GLU:H | 2.04 | 0.61 |
| 1:B:214:ARG:HA | 1:B:217:THR:CG2 | 2.30 | 0.61 |
| 1:A:214:ARG:HA | 1:A:217:THR:CG2 | 2.31 | 0.61 |
| 1:B:29:ALA:O | 1:B:31:TYR:N | 2.30 | 0.61 |
| 1:A:25:VAL:HG11 | 1:A:288:PRO:HA | 1.83 | 0.61 |
| 1:A:259:VAL:HG21 | 1:E:7:ARG:NH1 | 2.16 | 0.61 |
| 1:A:150:PRO:CA | 1:A:152:TYR:CE1 | 2.81 | 0.60 |
| 1:E:263:LEU:CD1 | 1:E:264:PRO:HD2 | 2.23 | 0.60 |
| 1:D:43:ASN:O | 1:D:44:THR:C | 2.38 | 0.60 |
| 1:C:199:ASP:HB2 | 1:C:217:THR:HG23 | 1.83 | 0.60 |
| 1:A:31:TYR:CD1 | 1:A:31:TYR:C | 2.73 | 0.60 |
| 1:B:66:ILE:O | 1:B:69:VAL:HG13 | 2.00 | 0.60 |
| 1:B:41:TYR:HE1 | 1:B:110:LEU:HD12 | 1.66 | 0.60 |
| 1:C:45:THR:C | 1:C:46:LYS:HD3 | 2.22 | 0.60 |
| 1:C:107:LEU:HD12 | 1:C:107:LEU:N | 2.16 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:398:LYS:HG2 | 1:A:402:MET:HE2 | 1.83 | 0.60 |
| 1:E:151:GLU:OE1 | 1:E:155:LYS:NZ | 2.35 | 0.60 |
| 1:A:81:ARG:CB | 1:A:208:HIS:HE2 | 2.14 | 0.60 |
| 1:B:302:GLN:HG2 | 1:B:316:ALA:CB | 2.31 | 0.60 |
| 1:B:153:ARG:NH1 | 1:B:176:PRO:C | 2.55 | 0.60 |
| 1:C:25:VAL:HG11 | 1:C:288:PRO:HA | 1.84 | 0.60 |
| 1:C:153:ARG:NH1 | 1:C:176:PRO:C | 2.54 | 0.60 |
| 1:D:89:SER:O | 1:D:90:SER:HB2 | 2.00 | 0.60 |
| 1:A:149:MET:O | 1:A:151:GLU:N | 2.34 | 0.60 |
| 1:B:150:PRO:HA | 1:B:152:TYR:CD1 | 2.36 | 0.60 |
| 1:E:317:ARG:CZ | 1:E:317:ARG:H | 2.14 | 0.60 |
| 1:C:317:ARG:NE | 1:C:317:ARG:N | 2.45 | 0.60 |
| 1:A:148:GLN:O | 1:A:152:TYR:HE2 | 1.85 | 0.60 |
| 1:B:184:VAL:HG13 | 1:C:165:LYS:HA | 1.84 | 0.60 |
| 1:A:344:LEU:HD13 | 1:E:250:LEU:HB3 | 1.83 | 0.60 |
| 1:C:180:ASP:OD2 | 1:D:164:CYS:HB3 | 2.00 | 0.60 |
| 2:R:11:C:H2' | 2:R:12:C:O4' | 2.02 | 0.60 |
| 1:E:31:TYR:C | 1:E:31:TYR:CD1 | 2.75 | 0.60 |
| 1:E:87:ASP:OD2 | 1:E:97:LYS:HG3 | 2.01 | 0.60 |
| 1:A:66:ILE:O | 1:A:69:VAL:HG13 | 2.01 | 0.60 |
| 1:E:165:LYS:O | 1:E:166:MET:HB2 | 2.01 | 0.59 |
| 2:R:12:C:C2' | 2:R:13:C:H5' | 2.31 | 0.59 |
| 1:B:165:LYS:NZ | 1:B:165:LYS:HB2 | 2.17 | 0.59 |
| 1:A:29:ALA:O | 1:A:31:TYR:N | 2.30 | 0.59 |
| 1:E:66:ILE:O | 1:E:69:VAL:HG13 | 2.02 | 0.59 |
| 1:D:352:ASP:OD1 | 1:D:352:ASP:C | 2.40 | 0.59 |
| 1:B:228:LEU:HB2 | 1:B:289:TYR:HB3 | 1.84 | 0.59 |
| 1:A:148:GLN:HG2 | 1:A:179:ARG:NH1 | 2.16 | 0.59 |
| 1:E:117:LEU:CB | 1:E:118:PRO:HD3 | 2.27 | 0.59 |
| 1:C:42:ILE:HD12 | 1:C:74:TYR:CD2 | 2.36 | 0.59 |
| 1:E:127:THR:HG23 | 1:E:129:ALA:H | 1.66 | 0.59 |
| 1:B:383:GLU:HG3 | 1:C:354:LYS:CE | 2.31 | 0.59 |
| 1:A:87:ASP:OD2 | 1:A:97:LYS:HG3 | 2.03 | 0.59 |
| 1:A:262:MET:HA | 1:A:262:MET:HE2 | 1.84 | 0.59 |
| 1:D:317:ARG:O | 1:D:319:PRO:HD3 | 2.02 | 0.59 |
| 1:C:214:ARG:HA | 1:C:217:THR:CG2 | 2.32 | 0.59 |
| 1:C:263:LEU:CD1 | 1:C:264:PRO:HD2 | 2.27 | 0.59 |
| 1:D:15:VAL:O | 1:D:17:LYS:HG2 | 2.03 | 0.59 |
| 1:B:226:ALA:O | 1:B:230:THR:HG23 | 2.02 | 0.59 |
| 1:A:169:GLU:HA | 1:A:170:GLN:NE2 | 2.17 | 0.59 |
| 1:E:228:LEU:HB2 | 1:E:289:TYR:HB3 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:25:VAL:HG11 | 1:D:288:PRO:HA | 1.85 | 0.58 |
| 1:D:66:ILE:O | 1:D:69:VAL:HG13 | 2.03 | 0.58 |
| 1:A:352:ASP:C | 1:A:352:ASP:OD1 | 2.42 | 0.58 |
| 1:C:50:ASP:OD2 | 1:C:120:GLY:HA2 | 2.03 | 0.58 |
| 1:C:262:MET:HE2 | 1:C:262:MET:HA | 1.84 | 0.58 |
| 1:B:22:GLU:HB3 | 1:C:206:LYS:NZ | 2.18 | 0.58 |
| 1:A:152:TYR:HD1 | 1:A:153:ARG:H | 1.51 | 0.58 |
| 1:B:148:GLN:O | 1:B:152:TYR:HE2 | 1.87 | 0.58 |
| 2:R:25:C:H2' | 2:R:26:C:C6 | 2.38 | 0.58 |
| 1:D:152:TYR:HD1 | 1:D:153:ARG:H | 1.52 | 0.58 |
| 1:A:106:ASP:C | 1:A:107:LEU:HD12 | 2.23 | 0.58 |
| 1:C:375:VAL:O | 1:C:379:LEU:HB2 | 2.03 | 0.58 |
| 1:B:68:HIS:HE1 | 1:B:117:LEU:HG | 1.67 | 0.58 |
| 1:D:412:ILE:C | 1:D:412:ILE:HD12 | 2.24 | 0.58 |
| 1:A:317:ARG:N | 1:A:317:ARG:NE | 2.50 | 0.58 |
| 1:B:22:GLU:HB3 | 1:C:206:LYS:HZ3 | 1.68 | 0.58 |
| 1:D:29:ALA:C | 1:D:31:TYR:H | 2.07 | 0.58 |
| 1:B:81:ARG:HB2 | 1:B:208:HIS:HE2 | 1.68 | 0.58 |
| 1:C:226:ALA:O | 1:C:230:THR:HG23 | 2.04 | 0.58 |
| 1:A:389:PRO:HA | 1:A:393:MET:CE | 2.34 | 0.58 |
| 1:B:29:ALA:C | 1:B:31:TYR:H | 2.08 | 0.58 |
| 1:B:127:THR:HG23 | 1:B:129:ALA:H | 1.69 | 0.58 |
| 1:C:150:PRO:CA | 1:C:152:TYR:CE1 | 2.83 | 0.57 |
| 1:A:150:PRO:HA | 1:A:152:TYR:CD1 | 2.38 | 0.57 |
| 1:D:107:LEU:HD12 | 1:D:107:LEU:N | 2.19 | 0.57 |
| 1:A:130:ASP:O | 1:A:132:LYS:N | 2.36 | 0.57 |
| 1:C:152:TYR:HD1 | 1:C:153:ARG:H | 1.52 | 0.57 |
| 1:E:130:ASP:O | 1:E:132:LYS:N | 2.36 | 0.57 |
| 1:B:87:ASP:OD2 | 1:B:97:LYS:HG3 | 2.05 | 0.57 |
| 1:C:66:ILE:O | 1:C:69:VAL:HG13 | 2.04 | 0.57 |
| 1:A:165:LYS:CB | 1:A:165:LYS:NZ | 2.67 | 0.57 |
| 1:D:317:ARG:NE | 1:D:317:ARG:N | 2.48 | 0.57 |
| 1:C:180:ASP:C | 1:C:180:ASP:OD2 | 2.43 | 0.57 |
| 1:A:14:ILE:HG23 | 1:A:16:PRO:HD3 | 1.87 | 0.57 |
| 1:D:178:GLY:O | 1:D:179:ARG:HB2 | 2.05 | 0.57 |
| 1:E:50:ASP:OD2 | 1:E:120:GLY:HA2 | 2.05 | 0.57 |
| 1:C:165:LYS:O | 1:C:166:MET:CB | 2.53 | 0.57 |
| 1:D:87:ASP:OD2 | 1:D:97:LYS:HG3 | 2.05 | 0.57 |
| 1:E:165:LYS:NZ | 1:E:165:LYS:HB2 | 2.18 | 0.57 |
| 1:E:224:ASP:CG | 2:R:39:C:H4' | 2.25 | 0.57 |
| 1:A:29:ALA:HB2 | 1:A:91:PHE:CE2 | 2.39 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:14:ILE:HD11 | 1:D:259:VAL:HA | 1.86 | 0.57 |
| 1:C:294:ASN:N | 1:C:295:PRO:HD3 | 2.20 | 0.57 |
| 2:R:21:C:C2' | 2:R:22:C:H5' | 2.35 | 0.57 |
| 1:C:383:GLU:HG3 | 1:D:354:LYS:HE2 | 1.86 | 0.57 |
| 1:C:106:ASP:C | 1:C:107:LEU:HD12 | 2.25 | 0.57 |
| 1:E:199:ASP:HB2 | 1:E:217:THR:HG23 | 1.86 | 0.57 |
| 1:C:14:ILE:HG23 | 1:C:16:PRO:HD3 | 1.87 | 0.57 |
| 1:C:342:ALA:HB1 | 1:C:344:LEU:HD23 | 1.87 | 0.57 |
| 1:C:292:VAL:HG12 | 2:R:13:C:H5 | 1.70 | 0.57 |
| 1:B:152:TYR:HD1 | 1:B:153:ARG:H | 1.53 | 0.57 |
| 1:A:117:LEU:HD23 | 1:A:117:LEU:N | 2.20 | 0.57 |
| 1:A:70:ASN:HD22 | 1:A:70:ASN:N | 2.03 | 0.57 |
| 1:D:143:ARG:NH1 | 2:R:9:C:H5' | 2.20 | 0.57 |
| 1:C:46:LYS:HD3 | 1:C:46:LYS:N | 2.19 | 0.57 |
| 1:D:171:PHE:CG | 1:D:172:GLU:N | 2.73 | 0.57 |
| 1:C:171:PHE:CG | 1:C:172:GLU:N | 2.72 | 0.57 |
| 1:E:262:MET:CE | 1:E:262:MET:HA | 2.35 | 0.57 |
| 1:A:323:GLU:OE1 | 1:B:239:GLY:HA3 | 2.05 | 0.57 |
| 1:D:27:TYR:HB3 | 1:D:266:GLN:HE22 | 1.68 | 0.56 |
| 1:D:215:TYR:HA | 2:R:9:C:O4' | 2.04 | 0.56 |
| 1:C:150:PRO:HA | 1:C:152:TYR:CD1 | 2.40 | 0.56 |
| 1:C:165:LYS:NZ | 1:C:165:LYS:CB | 2.67 | 0.56 |
| 1:A:199:ASP:OD1 | 1:A:217:THR:HG23 | 2.05 | 0.56 |
| 1:B:262:MET:HA | 1:B:262:MET:CE | 2.35 | 0.56 |
| 1:E:152:TYR:HD1 | 1:E:153:ARG:H | 1.53 | 0.56 |
| 1:D:106:ASP:C | 1:D:107:LEU:HD12 | 2.26 | 0.56 |
| 1:D:70:ASN:HD22 | 1:D:70:ASN:N | 2.04 | 0.56 |
| 1:D:81:ARG:HB2 | 1:D:208:HIS:HE2 | 1.70 | 0.56 |
| 1:A:171:PHE:CG | 1:A:172:GLU:N | 2.73 | 0.56 |
| 1:B:133:TRP:CB | 1:B:167:ILE:HD13 | 2.34 | 0.56 |
| 1:A:199:ASP:HB2 | 1:A:217:THR:HG23 | 1.87 | 0.56 |
| 1:C:89:SER:O | 1:C:90:SER:HB2 | 2.05 | 0.56 |
| 1:C:43:ASN:O | 1:C:44:THR:C | 2.43 | 0.56 |
| 1:C:117:LEU:HD23 | 1:C:117:LEU:N | 2.21 | 0.56 |
| 1:C:68:HIS:HE1 | 1:C:117:LEU:HG | 1.70 | 0.56 |
| 1:D:214:ARG:CA | 1:D:217:THR:HG22 | 2.35 | 0.56 |
| 1:E:58:GLY:O | 1:E:63:ASN:O | 2.24 | 0.56 |
| 1:C:199:ASP:CB | 1:C:217:THR:HG23 | 2.36 | 0.56 |
| 1:D:148:GLN:O | 1:D:152:TYR:CE2 | 2.59 | 0.56 |
| 2:R:40:C:H2' | 2:R:40:C:O2 | 2.04 | 0.56 |
| 1:B:45:THR:C | 1:B:46:LYS:HD3 | 2.26 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:143:ARG:HH12 | 2:R:9:C:C5' | 2.19 | 0.55 |
| 1:B:42:ILE:HD12 | 1:B:74:TYR:HD2 | 1.70 | 0.55 |
| 1:E:107:LEU:N | 1:E:107:LEU:HD12 | 2.21 | 0.55 |
| 1:D:150:PRO:CA | 1:D:152:TYR:CE1 | 2.86 | 0.55 |
| 1:A:42:ILE:HD12 | 1:A:74:TYR:HD2 | 1.72 | 0.55 |
| 1:A:165:LYS:O | 1:A:167:ILE:CD1 | 2.48 | 0.55 |
| 1:D:68:HIS:HE1 | 1:D:117:LEU:HG | 1.71 | 0.55 |
| 1:C:29:ALA:C | 1:C:31:TYR:H | 2.08 | 0.55 |
| 1:B:178:GLY:O | 1:B:179:ARG:HB2 | 2.05 | 0.55 |
| 1:A:68:HIS:HE1 | 1:A:117:LEU:HG | 1.70 | 0.55 |
| 1:D:45:THR:C | 1:D:46:LYS:HD3 | 2.27 | 0.55 |
| 1:B:163:GLN:O | 1:B:167:ILE:HD12 | 2.05 | 0.55 |
| 1:E:29:ALA:O | 1:E:31:TYR:N | 2.33 | 0.55 |
| 1:C:127:THR:HG23 | 1:C:129:ALA:H | 1.70 | 0.55 |
| 1:E:150:PRO:CA | 1:E:152:TYR:CE1 | 2.87 | 0.55 |
| 1:C:167:ILE:O | 1:C:168:ASN:C | 2.44 | 0.55 |
| 1:D:136:LEU:C | 1:D:136:LEU:HD23 | 2.27 | 0.55 |
| 1:A:199:ASP:CB | 1:A:217:THR:HG23 | 2.36 | 0.55 |
| 1:C:36:LYS:HG3 | 1:C:93:ILE:HD11 | 1.89 | 0.55 |
| 1:E:148:GLN:O | 1:E:152:TYR:HE2 | 1.90 | 0.55 |
| 1:E:178:GLY:O | 1:E:179:ARG:HB2 | 2.06 | 0.55 |
| 1:D:224:ASP:CG | 2:R:3:C:H4' | 2.27 | 0.55 |
| 1:D:166:MET:C | 1:D:167:ILE:HG13 | 2.25 | 0.55 |
| 1:D:262:MET:HA | 1:D:262:MET:CE | 2.36 | 0.55 |
| 1:E:389:PRO:HA | 1:E:393:MET:CE | 2.37 | 0.55 |
| 1:E:14:ILE:HG23 | 1:E:16:PRO:HD3 | 1.89 | 0.55 |
| 1:E:68:HIS:HE1 | 1:E:117:LEU:HG | 1.70 | 0.55 |
| 1:D:165:LYS:NZ | 1:D:165:LYS:HB2 | 2.22 | 0.55 |
| 1:B:42:ILE:HD12 | 1:B:74:TYR:CD2 | 2.42 | 0.55 |
| 1:B:171:PHE:HZ | 1:B:173:PRO:HG2 | 1.72 | 0.55 |
| 1:B:15:VAL:O | 1:B:17:LYS:HG2 | 2.07 | 0.55 |
| 1:A:58:GLY:O | 1:A:63:ASN:O | 2.24 | 0.55 |
| 2:R:16:C:H2' | 2:R:17:C:C6 | 2.42 | 0.54 |
| 1:B:117:LEU:N | 1:B:117:LEU:HD23 | 2.21 | 0.54 |
| 1:B:350:VAL:HG13 | 1:E:4:THR:O | 2.07 | 0.54 |
| 1:A:166:MET:H | 1:E:184:VAL:CG1 | 2.18 | 0.54 |
| 1:A:167:ILE:HG22 | 1:A:169:GLU:OE1 | 2.07 | 0.54 |
| 1:A:214:ARG:CA | 1:A:217:THR:HG22 | 2.37 | 0.54 |
| 1:B:365:THR:HG23 | 1:B:366:THR:H | 1.72 | 0.54 |
| 1:B:385:GLN:HG2 | 1:B:390:THR:HG22 | 1.89 | 0.54 |
| 1:E:294:ASN:N | 1:E:295:PRO:HD3 | 2.22 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:203:HIS:O | 1:B:206:LYS:HG3 | 2.07 | 0.54 |
| 1:A:385:GLN:HG2 | 1:A:390:THR:HG22 | 1.89 | 0.54 |
| 1:C:70:ASN:HD22 | 1:C:70:ASN:N | 2.05 | 0.54 |
| 1:A:180:ASP:OD2 | 1:A:180:ASP:C | 2.44 | 0.54 |
| 1:C:385:GLN:HG2 | 1:C:390:THR:HG22 | 1.90 | 0.54 |
| 1:B:43:ASN:OD1 | 1:B:112:ALA:N | 2.41 | 0.54 |
| 1:C:167:ILE:O | 1:C:169:GLU:CD | 2.46 | 0.54 |
| 1:D:42:ILE:HD12 | 1:D:74:TYR:HD2 | 1.73 | 0.54 |
| 1:E:214:ARG:CA | 1:E:217:THR:HG22 | 2.37 | 0.54 |
| 1:E:29:ALA:C | 1:E:31:TYR:H | 2.11 | 0.54 |
| 1:B:81:ARG:HD2 | 1:B:208:HIS:HE2 | 1.73 | 0.54 |
| 1:D:70:ASN:HD22 | 1:D:70:ASN:H | 1.55 | 0.54 |
| 1:D:398:LYS:HG2 | 1:D:402:MET:HE2 | 1.90 | 0.54 |
| 2:R:12:C:H2' | 2:R:13:C:H5' | 1.89 | 0.54 |
| 1:A:153:ARG:NH1 | 1:A:176:PRO:O | 2.39 | 0.54 |
| 1:D:42:ILE:HD12 | 1:D:74:TYR:CD2 | 2.43 | 0.54 |
| 1:D:130:ASP:O | 1:D:132:LYS:N | 2.36 | 0.54 |
| 1:D:385:GLN:HG2 | 1:D:390:THR:HG22 | 1.90 | 0.54 |
| 1:D:150:PRO:HA | 1:D:152:TYR:CD1 | 2.41 | 0.54 |
| 1:C:43:ASN:OD1 | 1:C:112:ALA:N | 2.41 | 0.54 |
| 1:C:203:HIS:O | 1:C:206:LYS:HG3 | 2.08 | 0.54 |
| 1:D:203:HIS:O | 1:D:206:LYS:HG3 | 2.07 | 0.54 |
| 1:E:70:ASN:N | 1:E:70:ASN:HD22 | 2.05 | 0.54 |
| 1:C:178:GLY:O | 1:C:179:ARG:HB2 | 2.08 | 0.54 |
| 1:A:42:ILE:HD12 | 1:A:74:TYR:CD2 | 2.43 | 0.54 |
| 1:E:42:ILE:HD12 | 1:E:74:TYR:HD2 | 1.73 | 0.54 |
| 1:B:130:ASP:O | 1:B:132:LYS:N | 2.39 | 0.54 |
| 1:E:171:PHE:CG | 1:E:172:GLU:N | 2.74 | 0.54 |
| 1:B:295:PRO:HB2 | 1:B:322:ILE:CG2 | 2.38 | 0.54 |
| 1:B:150:PRO:HD3 | 1:B:152:TYR:OH | 2.08 | 0.54 |
| 1:E:106:ASP:C | 1:E:107:LEU:HD12 | 2.28 | 0.54 |
| 1:C:130:ASP:O | 1:C:132:LYS:N | 2.38 | 0.54 |
| 1:C:203:HIS:HD2 | 1:C:272:ASP:OD1 | 1.89 | 0.54 |
| 1:E:167:ILE:HG22 | 1:E:168:ASN:N | 2.22 | 0.54 |
| 1:B:214:ARG:CA | 1:B:217:THR:HG22 | 2.38 | 0.54 |
| 1:C:309:ARG:HD2 | 1:C:309:ARG:N | 2.23 | 0.54 |
| 1:E:352:ASP:C | 1:E:352:ASP:OD1 | 2.46 | 0.54 |
| 1:E:412:ILE:C | 1:E:412:ILE:HD12 | 2.27 | 0.54 |
| 1:E:359:ASP:O | 1:E:361:THR:HG23 | 2.07 | 0.54 |
| 1:A:243:GLU:HG3 | 1:E:2:SER:O | 2.08 | 0.54 |
| 1:C:87:ASP:OD2 | 1:C:97:LYS:HG3 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:308:LEU:O | 1:C:309:ARG:HB2 | 2.08 | 0.54 |
| 1:B:5:VAL:CG1 | 1:D:348:PHE:HB3 | 2.38 | 0.54 |
| 1:A:50:ASP:OD2 | 1:A:120:GLY:HA2 | 2.08 | 0.53 |
| 1:B:46:LYS:HD3 | 1:B:46:LYS:N | 2.21 | 0.53 |
| 1:E:81:ARG:HB2 | 1:E:208:HIS:HE2 | 1.72 | 0.53 |
| 1:C:385:GLN:O | 1:C:386:ASN:HB2 | 2.08 | 0.53 |
| 1:D:147:THR:HG21 | 1:D:152:TYR:HB3 | 1.89 | 0.53 |
| 1:A:323:GLU:O | 1:A:327:LEU:HD22 | 2.08 | 0.53 |
| 1:A:165:LYS:HZ2 | 1:A:165:LYS:HB2 | 1.71 | 0.53 |
| 1:B:136:LEU:HD23 | 1:B:136:LEU:C | 2.28 | 0.53 |
| 1:B:389:PRO:HA | 1:B:393:MET:CE | 2.38 | 0.53 |
| 1:C:148:GLN:O | 1:C:152:TYR:HE2 | 1.91 | 0.53 |
| 1:D:60:LYS:O | 1:D:61:SER:CB | 2.46 | 0.53 |
| 1:E:308:LEU:O | 1:E:309:ARG:HB2 | 2.09 | 0.53 |
| 1:A:294:ASN:N | 1:A:295:PRO:HD3 | 2.23 | 0.53 |
| 1:C:38:ILE:HD11 | 1:C:107:LEU:O | 2.09 | 0.53 |
| 1:E:385:GLN:HG2 | 1:E:390:THR:HG22 | 1.89 | 0.53 |
| 1:B:70:ASN:N | 1:B:70:ASN:HD22 | 2.07 | 0.53 |
| 1:D:309:ARG:N | 1:D:309:ARG:HD2 | 2.24 | 0.53 |
| 1:E:323:GLU:O | 1:E:327:LEU:HD22 | 2.09 | 0.53 |
| 1:E:166:MET:HB2 | 1:E:167:ILE:HG13 | 1.89 | 0.53 |
| 1:E:149:MET:C | 1:E:151:GLU:N | 2.62 | 0.53 |
| 1:C:172:GLU:HB3 | 1:C:173:PRO:CD | 2.39 | 0.53 |
| 1:C:389:PRO:HA | 1:C:393:MET:CE | 2.37 | 0.53 |
| 1:E:150:PRO:HA | 1:E:152:TYR:CD1 | 2.43 | 0.53 |
| 1:A:370:PRO:HD3 | 1:A:381:TRP:CG | 2.44 | 0.53 |
| 1:D:117:LEU:HD23 | 1:D:117:LEU:N | 2.24 | 0.53 |
| 1:B:27:TYR:HB3 | 1:B:266:GLN:HE22 | 1.73 | 0.53 |
| 1:B:294:ASN:N | 1:B:295:PRO:HD3 | 2.24 | 0.53 |
| 1:A:203:HIS:HD2 | 1:A:272:ASP:OD1 | 1.91 | 0.53 |
| 1:B:230:THR:HG21 | 1:B:298:HIS:ND1 | 2.22 | 0.53 |
| 1:E:45:THR:H | 1:E:111:LYS:NZ | 2.07 | 0.53 |
| 1:E:199:ASP:CB | 1:E:217:THR:HG23 | 2.38 | 0.53 |
| 1:E:45:THR:C | 1:E:46:LYS:HD3 | 2.29 | 0.52 |
| 1:D:81:ARG:HD2 | 1:D:208:HIS:HE2 | 1.74 | 0.52 |
| 1:A:203:HIS:O | 1:A:206:LYS:HG3 | 2.09 | 0.52 |
| 1:B:45:THR:H | 1:B:111:LYS:NZ | 2.06 | 0.52 |
| 1:E:104:ILE:O | 1:E:107:LEU:HD13 | 2.10 | 0.52 |
| 1:A:398:LYS:HG2 | 1:A:402:MET:CE | 2.39 | 0.52 |
| 1:D:230:THR:HG21 | 1:D:298:HIS:ND1 | 2.24 | 0.52 |
| 1:D:203:HIS:HD2 | 1:D:272:ASP:OD1 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:203:HIS:O | 1:E:206:LYS:HG3 | 2.09 | 0.52 |
| 1:E:230:THR:HG21 | 1:E:298:HIS:ND1 | 2.24 | 0.52 |
| 1:B:54:TYR:CD1 | 1:B:122:SER:HB2 | 2.45 | 0.52 |
| 1:C:165:LYS:O | 1:C:167:ILE:HG12 | 2.08 | 0.52 |
| 1:A:130:ASP:C | 1:A:132:LYS:N | 2.63 | 0.52 |
| 1:A:402:MET:SD | 1:E:422:LYS:HD2 | 2.49 | 0.52 |
| 1:D:308:LEU:O | 1:D:309:ARG:HB2 | 2.10 | 0.52 |
| 1:B:308:LEU:O | 1:B:309:ARG:HB2 | 2.08 | 0.52 |
| 1:B:223:LYS:O | 1:B:224:ASP:HB2 | 2.09 | 0.52 |
| 1:B:31:TYR:C | 1:B:33:ARG:H | 2.12 | 0.52 |
| 1:C:31:TYR:C | 1:C:33:ARG:H | 2.13 | 0.52 |
| 1:E:169:GLU:CG | 1:E:170:GLN:N | 2.60 | 0.52 |
| 1:D:149:MET:C | 1:D:151:GLU:N | 2.62 | 0.52 |
| 1:C:136:LEU:C | 1:C:136:LEU:HD23 | 2.29 | 0.52 |
| 1:D:253:GLU:N | 1:D:253:GLU:OE2 | 2.41 | 0.52 |
| 2:R:27:C:C2' | 2:R:28:C:O5' | 2.58 | 0.52 |
| 1:E:163:GLN:O | 1:E:167:ILE:HD12 | 2.10 | 0.52 |
| 1:A:298:HIS:NE2 | 1:A:317:ARG:NH1 | 2.58 | 0.52 |
| 1:C:151:GLU:O | 1:C:155:LYS:HB2 | 2.09 | 0.52 |
| 1:A:43:ASN:OD1 | 1:A:112:ALA:N | 2.42 | 0.52 |
| 1:A:31:TYR:C | 1:A:33:ARG:H | 2.13 | 0.52 |
| 1:A:309:ARG:HD2 | 1:A:309:ARG:N | 2.25 | 0.52 |
| 1:D:294:ASN:N | 1:D:295:PRO:HD3 | 2.25 | 0.52 |
| 1:A:178:GLY:O | 1:A:179:ARG:HB2 | 2.08 | 0.51 |
| 1:D:389:PRO:HA | 1:D:393:MET:CE | 2.40 | 0.51 |
| 1:B:253:GLU:OE2 | 1:B:253:GLU:N | 2.39 | 0.51 |
| 1:B:370:PRO:HD3 | 1:B:381:TRP:CG | 2.45 | 0.51 |
| 1:D:370:PRO:HD3 | 1:D:381:TRP:CG | 2.45 | 0.51 |
| 1:E:317:ARG:NE | 1:E:317:ARG:N | 2.56 | 0.51 |
| 1:E:54:TYR:CD1 | 1:E:122:SER:HB2 | 2.46 | 0.51 |
| 1:C:45:THR:H | 1:C:111:LYS:NZ | 2.07 | 0.51 |
| 1:D:59:LEU:O | 1:D:61:SER:N | 2.42 | 0.51 |
| 1:E:130:ASP:C | 1:E:132:LYS:N | 2.62 | 0.51 |
| 1:C:342:ALA:CB | 1:C:344:LEU:HD23 | 2.39 | 0.51 |
| 1:B:309:ARG:N | 1:B:309:ARG:HD2 | 2.25 | 0.51 |
| 1:E:36:LYS:HG3 | 1:E:93:ILE:HD11 | 1.92 | 0.51 |
| 1:C:81:ARG:HD2 | 1:C:208:HIS:HE2 | 1.74 | 0.51 |
| 1:D:180:ASP:C | 1:D:180:ASP:OD2 | 2.48 | 0.51 |
| 1:B:298:HIS:NE2 | 1:B:317:ARG:NH1 | 2.59 | 0.51 |
| 1:A:149:MET:O | 1:A:152:TYR:CD2 | 2.64 | 0.51 |
| 1:B:149:MET:C | 1:B:151:GLU:N | 2.64 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:54:TYR:CD1 | 1:D:122:SER:HB2 | 2.46 | 0.51 |
| 1:E:61:SER:O | 1:E:63:ASN:N | 2.38 | 0.51 |
| 1:E:59:LEU:HB3 | 1:E:172:GLU:HG2 | 1.93 | 0.51 |
| 1:C:370:PRO:HD3 | 1:C:381:TRP:CG | 2.45 | 0.51 |
| 1:A:148:GLN:O | 1:A:152:TYR:CE2 | 2.62 | 0.51 |
| 1:B:72:TYR:O | 1:B:72:TYR:CD2 | 2.63 | 0.51 |
| 1:C:72:TYR:CD2 | 1:C:72:TYR:O | 2.63 | 0.51 |
| 1:B:398:LYS:HG2 | 1:B:402:MET:CE | 2.41 | 0.51 |
| 1:C:81:ARG:HB2 | 1:C:208:HIS:HE2 | 1.72 | 0.51 |
| 1:A:81:ARG:HD2 | 1:A:208:HIS:HE2 | 1.76 | 0.51 |
| 1:E:295:PRO:HB2 | 1:E:322:ILE:CG2 | 2.40 | 0.51 |
| 2:R:27:C:H2' | 2:R:28:C:O5' | 2.11 | 0.51 |
| 1:E:298:HIS:NE2 | 1:E:317:ARG:NH1 | 2.59 | 0.51 |
| 1:C:54:TYR:CD1 | 1:C:122:SER:HB2 | 2.45 | 0.51 |
| 1:C:184:VAL:HG13 | 1:D:165:LYS:CG | 2.40 | 0.51 |
| 1:C:27:TYR:HB3 | 1:C:266:GLN:HE22 | 1.74 | 0.51 |
| 1:E:81:ARG:HD2 | 1:E:208:HIS:HE2 | 1.74 | 0.51 |
| 1:B:14:ILE:HG23 | 1:B:16:PRO:HD3 | 1.93 | 0.51 |
| 1:D:147:THR:CG2 | 1:D:152:TYR:HB3 | 2.41 | 0.51 |
| 1:C:149:MET:HB3 | 1:C:150:PRO:HD2 | 1.92 | 0.51 |
| 1:B:149:MET:C | 1:B:152:TYR:CE2 | 2.84 | 0.51 |
| 1:B:171:PHE:HE2 | 1:B:173:PRO:O | 1.94 | 0.51 |
| 1:E:309:ARG:HD2 | 1:E:309:ARG:N | 2.26 | 0.51 |
| 1:A:308:LEU:O | 1:A:309:ARG:HB2 | 2.10 | 0.51 |
| 1:D:408:ARG:NH2 | 2:R:6:C:H2' | 2.26 | 0.51 |
| 1:C:147:THR:HG21 | 1:C:152:TYR:HB3 | 1.92 | 0.51 |
| 1:C:214:ARG:CA | 1:C:217:THR:HG22 | 2.40 | 0.51 |
| 1:C:199:ASP:OD1 | 1:C:217:THR:HG23 | 2.10 | 0.51 |
| 1:A:342:ALA:HB1 | 1:A:344:LEU:HD23 | 1.93 | 0.51 |
| 1:E:151:GLU:O | 1:E:155:LYS:HB2 | 2.10 | 0.51 |
| 1:D:72:TYR:CD2 | 1:D:72:TYR:C | 2.82 | 0.51 |
| 1:D:199:ASP:HB2 | 1:D:217:THR:HG23 | 1.91 | 0.51 |
| 1:A:136:LEU:HD23 | 1:A:136:LEU:C | 2.32 | 0.51 |
| 1:B:171:PHE:CE2 | 1:B:173:PRO:O | 2.64 | 0.51 |
| 1:D:130:ASP:C | 1:D:132:LYS:N | 2.62 | 0.51 |
| 1:C:323:GLU:O | 1:C:327:LEU:HD22 | 2.10 | 0.51 |
| 1:E:15:VAL:O | 1:E:17:LYS:HG2 | 2.11 | 0.51 |
| 1:E:147:THR:HG21 | 1:E:152:TYR:HB3 | 1.93 | 0.51 |
| 1:A:383:GLU:HG3 | 1:B:354:LYS:CE | 2.41 | 0.51 |
| 1:A:54:TYR:CD1 | 1:A:122:SER:HB2 | 2.46 | 0.51 |
| 1:A:45:THR:C | 1:A:46:LYS:HD3 | 2.30 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:42:ILE:HD12 | 1:E:74:TYR:CD2 | 2.45 | 0.51 |
| 1:D:401:VAL:HG21 | 1:D:420:PHE:HB2 | 1.92 | 0.51 |
| 1:A:147:THR:HG21 | 1:A:152:TYR:HB3 | 1.91 | 0.50 |
| 1:A:149:MET:HB3 | 1:A:150:PRO:HD2 | 1.93 | 0.50 |
| 1:D:72:TYR:CD2 | 1:D:72:TYR:O | 2.63 | 0.50 |
| 2:R:18:C:O2' | 2:R:19:C:H5' | 2.11 | 0.50 |
| 1:A:41:TYR:CE1 | 1:A:110:LEU:HD12 | 2.45 | 0.50 |
| 1:E:233:HIS:HB2 | 1:E:312:ARG:NH1 | 2.26 | 0.50 |
| 1:E:180:ASP:OD2 | 1:E:180:ASP:C | 2.49 | 0.50 |
| 1:C:155:LYS:NZ | 2:R:17:C:OP2 | 2.39 | 0.50 |
| 1:D:316:ALA:HA | 1:D:317:ARG:CZ | 2.41 | 0.50 |
| 1:C:184:VAL:HG11 | 1:D:166:MET:H | 1.76 | 0.50 |
| 1:D:31:TYR:C | 1:D:33:ARG:H | 2.14 | 0.50 |
| 1:E:70:ASN:HD22 | 1:E:70:ASN:H | 1.58 | 0.50 |
| 1:B:323:GLU:OE1 | 1:C:239:GLY:HA3 | 2.11 | 0.50 |
| 1:E:177:GLU:HG2 | 1:E:178:GLY:N | 2.26 | 0.50 |
| 1:E:253:GLU:N | 1:E:253:GLU:OE2 | 2.41 | 0.50 |
| 1:E:172:GLU:HB3 | 1:E:173:PRO:CD | 2.41 | 0.50 |
| 2:R:10:C:H5'' | 2:R:11:C:OP2 | 2.11 | 0.50 |
| 2:R:34:C:O4' | 2:R:34:C:O2 | 2.28 | 0.50 |
| 1:B:323:GLU:O | 1:B:327:LEU:HD22 | 2.11 | 0.50 |
| 1:A:218:ILE:C | 1:A:220:SER:H | 2.15 | 0.50 |
| 1:E:354:LYS:CE | 1:E:356:THR:HA | 2.33 | 0.50 |
| 1:B:199:ASP:HB2 | 1:B:217:THR:HG23 | 1.93 | 0.50 |
| 1:C:295:PRO:HB2 | 1:C:322:ILE:CG2 | 2.41 | 0.50 |
| 1:D:328:THR:HG21 | 1:D:415:TYR:OH | 2.11 | 0.50 |
| 1:C:181:ILE:CD1 | 1:C:181:ILE:H | 2.17 | 0.50 |
| 1:B:151:GLU:O | 1:B:155:LYS:HB2 | 2.12 | 0.50 |
| 1:B:72:TYR:CD2 | 1:B:72:TYR:C | 2.82 | 0.50 |
| 1:A:172:GLU:HB3 | 1:A:173:PRO:CD | 2.42 | 0.50 |
| 1:C:60:LYS:O | 1:C:61:SER:CB | 2.52 | 0.50 |
| 1:E:136:LEU:C | 1:E:136:LEU:HD23 | 2.32 | 0.49 |
| 1:C:230:THR:HG21 | 1:C:298:HIS:ND1 | 2.26 | 0.49 |
| 1:A:230:THR:HG21 | 1:A:298:HIS:ND1 | 2.27 | 0.49 |
| 1:B:184:VAL:CG1 | 1:C:165:LYS:HA | 2.41 | 0.49 |
| 1:A:262:MET:HA | 1:A:262:MET:CE | 2.42 | 0.49 |
| 1:B:240:MET:HE3 | 1:B:244:ASP:HB3 | 1.94 | 0.49 |
| 1:A:314:ARG:O | 1:A:413:GLY:HA3 | 2.12 | 0.49 |
| 1:C:72:TYR:CD2 | 1:C:72:TYR:C | 2.83 | 0.49 |
| 1:B:105:PHE:C | 1:B:107:LEU:N | 2.66 | 0.49 |
| 1:E:91:PHE:CE2 | 1:E:267:GLU:HG3 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:81:ARG:HB2 | 1:A:208:HIS:HE2 | 1.75 | 0.49 |
| 1:E:153:ARG:NH1 | 1:E:176:PRO:O | 2.45 | 0.49 |
| 1:D:179:ARG:HA | 1:D:183:ASP:OD1 | 2.12 | 0.49 |
| 1:A:177:GLU:HG2 | 1:A:178:GLY:N | 2.27 | 0.49 |
| 1:B:68:HIS:CE1 | 1:B:117:LEU:HG | 2.46 | 0.49 |
| 1:E:65:SER:HB3 | 1:E:68:HIS:ND1 | 2.27 | 0.49 |
| 1:D:170:GLN:O | 1:D:171:PHE:HB3 | 2.13 | 0.49 |
| 1:B:199:ASP:CB | 1:B:217:THR:HG23 | 2.41 | 0.49 |
| 1:B:14:ILE:HD11 | 1:C:259:VAL:HA | 1.94 | 0.49 |
| 1:E:203:HIS:HD2 | 1:E:272:ASP:OD1 | 1.94 | 0.49 |
| 1:E:149:MET:HB3 | 1:E:150:PRO:HD2 | 1.95 | 0.49 |
| 1:E:38:ILE:HD11 | 1:E:107:LEU:O | 2.12 | 0.49 |
| 1:B:37:GLU:HB2 | 1:B:108:VAL:HG21 | 1.95 | 0.49 |
| 1:D:38:ILE:HD11 | 1:D:107:LEU:O | 2.11 | 0.49 |
| 1:C:293:LYS:C | 1:C:295:PRO:HD3 | 2.32 | 0.49 |
| 1:E:370:PRO:HD3 | 1:E:381:TRP:CG | 2.47 | 0.49 |
| 1:D:141:LEU:HD22 | 1:D:182:PHE:CE1 | 2.47 | 0.49 |
| 1:A:149:MET:C | 1:A:151:GLU:N | 2.66 | 0.49 |
| 1:B:177:GLU:HG2 | 1:B:178:GLY:N | 2.28 | 0.49 |
| 1:A:165:LYS:HG3 | 1:E:184:VAL:HG13 | 1.94 | 0.49 |
| 1:D:43:ASN:OD1 | 1:D:112:ALA:N | 2.46 | 0.49 |
| 1:D:298:HIS:NE2 | 1:D:317:ARG:NH1 | 2.59 | 0.49 |
| 1:D:41:TYR:CE1 | 1:D:110:LEU:HD12 | 2.43 | 0.49 |
| 1:B:379:LEU:CD1 | 1:C:346:GLN:HB2 | 2.42 | 0.49 |
| 1:C:233:HIS:HB2 | 1:C:312:ARG:NH1 | 2.27 | 0.49 |
| 1:D:8:ILE:O | 1:D:8:ILE:HG13 | 2.13 | 0.49 |
| 1:A:151:GLU:O | 1:A:155:LYS:HB2 | 2.12 | 0.49 |
| 1:D:122:SER:O | 1:D:123:ASP:HB2 | 2.10 | 0.49 |
| 1:D:230:THR:HB | 1:D:302:GLN:OE1 | 2.12 | 0.49 |
| 1:E:8:ILE:HG13 | 1:E:8:ILE:O | 2.11 | 0.49 |
| 1:A:364:LEU:O | 1:A:365:THR:C | 2.50 | 0.49 |
| 1:B:149:MET:O | 1:B:152:TYR:CD2 | 2.65 | 0.49 |
| 1:A:72:TYR:CD2 | 1:A:72:TYR:O | 2.65 | 0.49 |
| 1:E:117:LEU:HD23 | 1:E:117:LEU:N | 2.28 | 0.49 |
| 1:A:45:THR:H | 1:A:111:LYS:HZ1 | 1.61 | 0.49 |
| 1:D:172:GLU:HB3 | 1:D:173:PRO:CD | 2.42 | 0.49 |
| 1:A:385:GLN:O | 1:A:386:ASN:HB2 | 2.13 | 0.49 |
| 1:C:412:ILE:HD12 | 1:C:412:ILE:C | 2.32 | 0.49 |
| 1:C:177:GLU:HG2 | 1:C:178:GLY:N | 2.28 | 0.49 |
| 1:A:150:PRO:HD3 | 1:A:152:TYR:OH | 2.12 | 0.49 |
| 1:A:149:MET:C | 1:A:152:TYR:CE2 | 2.85 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:122:SER:O | 1:A:123:ASP:HB2 | 2.12 | 0.49 |
| 1:E:46:LYS:HD3 | 1:E:46:LYS:N | 2.26 | 0.49 |
| 1:C:130:ASP:C | 1:C:132:LYS:N | 2.65 | 0.49 |
| 1:A:239:GLY:HA3 | 1:E:323:GLU:OE1 | 2.12 | 0.49 |
| 1:D:212:SER:HA | 2:R:9:C:O2 | 2.12 | 0.49 |
| 1:E:72:TYR:CD2 | 1:E:72:TYR:O | 2.66 | 0.49 |
| 1:B:54:TYR:CD1 | 1:B:118:PRO:HB2 | 2.48 | 0.49 |
| 1:A:38:ILE:HD11 | 1:A:107:LEU:O | 2.13 | 0.49 |
| 1:A:27:TYR:HB3 | 1:A:266:GLN:HE22 | 1.78 | 0.49 |
| 1:C:223:LYS:O | 1:C:224:ASP:HB2 | 2.13 | 0.49 |
| 1:B:122:SER:O | 1:B:123:ASP:HB2 | 2.12 | 0.48 |
| 1:B:354:LYS:CE | 1:B:356:THR:HA | 2.37 | 0.48 |
| 1:B:376:VAL:HG13 | 1:C:354:LYS:CB | 2.39 | 0.48 |
| 1:D:165:LYS:O | 1:D:167:ILE:CD1 | 2.58 | 0.48 |
| 1:E:37:GLU:HB2 | 1:E:108:VAL:HG21 | 1.95 | 0.48 |
| 1:B:130:ASP:C | 1:B:132:LYS:N | 2.65 | 0.48 |
| 1:D:295:PRO:HB2 | 1:D:322:ILE:CG2 | 2.43 | 0.48 |
| 1:A:15:VAL:O | 1:A:17:LYS:HG2 | 2.12 | 0.48 |
| 1:B:317:ARG:CD | 1:B:317:ARG:H | 2.25 | 0.48 |
| 1:C:141:LEU:HD22 | 1:C:182:PHE:CE1 | 2.47 | 0.48 |
| 1:E:43:ASN:OD1 | 1:E:112:ALA:N | 2.46 | 0.48 |
| 1:D:199:ASP:CB | 1:D:217:THR:HG23 | 2.43 | 0.48 |
| 2:R:18:C:C6 | 2:R:18:C:H5' | 2.48 | 0.48 |
| 1:C:166:MET:HB2 | 1:C:167:ILE:CD1 | 2.43 | 0.48 |
| 1:C:180:ASP:O | 1:C:180:ASP:OD2 | 2.31 | 0.48 |
| 1:A:241:SER:OG | 1:A:243:GLU:HG2 | 2.14 | 0.48 |
| 1:A:295:PRO:HB2 | 1:A:322:ILE:CG2 | 2.42 | 0.48 |
| 1:B:240:MET:HE3 | 1:B:244:ASP:CB | 2.42 | 0.48 |
| 1:C:401:VAL:HG21 | 1:C:420:PHE:HB2 | 1.94 | 0.48 |
| 1:D:151:GLU:O | 1:D:155:LYS:HB2 | 2.13 | 0.48 |
| 1:B:179:ARG:HA | 1:B:183:ASP:OD1 | 2.12 | 0.48 |
| 1:C:356:THR:CG2 | 1:C:357:PRO:HD3 | 2.29 | 0.48 |
| 1:C:37:GLU:HB2 | 1:C:108:VAL:HG21 | 1.95 | 0.48 |
| 1:B:148:GLN:O | 1:B:152:TYR:CE2 | 2.65 | 0.48 |
| 1:B:149:MET:HB3 | 1:B:150:PRO:HD2 | 1.95 | 0.48 |
| 1:C:380:GLY:CA | 1:D:354:LYS:HZ3 | 2.25 | 0.48 |
| 1:E:122:SER:O | 1:E:123:ASP:HB2 | 2.12 | 0.48 |
| 1:C:68:HIS:CE1 | 1:C:117:LEU:HG | 2.48 | 0.48 |
| 1:B:165:LYS:HB2 | 1:B:165:LYS:HZ2 | 1.78 | 0.48 |
| 1:C:262:MET:HA | 1:C:262:MET:CE | 2.43 | 0.48 |
| 1:B:36:LYS:HG3 | 1:B:93:ILE:HD11 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:18:LEU:HD12 | 1:B:232:GLY:HA2 | 1.95 | 0.48 |
| 2:R:44:C:H5'' | 2:R:45:C:OP2 | 2.12 | 0.48 |
| 1:D:68:HIS:CE1 | 1:D:118:PRO:HD2 | 2.49 | 0.48 |
| 1:B:253:GLU:HA | 1:B:256:ASP:HB2 | 1.95 | 0.48 |
| 1:B:385:GLN:O | 1:B:386:ASN:HB2 | 2.14 | 0.48 |
| 1:D:149:MET:HB3 | 1:D:150:PRO:HD2 | 1.95 | 0.48 |
| 1:B:147:THR:HG21 | 1:B:152:TYR:HB3 | 1.94 | 0.48 |
| 1:A:165:LYS:CB | 1:A:165:LYS:HZ3 | 2.27 | 0.48 |
| 1:A:253:GLU:HA | 1:A:256:ASP:HB2 | 1.95 | 0.48 |
| 1:C:238:THR:C | 1:C:240:MET:H | 2.16 | 0.48 |
| 1:B:180:ASP:OD2 | 1:B:180:ASP:C | 2.50 | 0.48 |
| 1:E:147:THR:CG2 | 1:E:152:TYR:HB3 | 2.44 | 0.48 |
| 1:C:59:LEU:HB3 | 1:C:172:GLU:HG2 | 1.96 | 0.48 |
| 1:E:255:ALA:O | 1:E:259:VAL:HG23 | 2.14 | 0.48 |
| 1:A:293:LYS:C | 1:A:295:PRO:HD3 | 2.35 | 0.48 |
| 1:A:412:ILE:HD12 | 1:A:412:ILE:C | 2.34 | 0.48 |
| 1:B:317:ARG:NE | 2:R:22:C:O2' | 2.47 | 0.48 |
| 1:D:68:HIS:CE1 | 1:D:117:LEU:HG | 2.49 | 0.48 |
| 1:C:136:LEU:HD23 | 1:C:136:LEU:O | 2.14 | 0.48 |
| 1:B:199:ASP:OD1 | 1:B:217:THR:HG23 | 2.13 | 0.48 |
| 1:C:283:LEU:N | 1:C:283:LEU:HD23 | 2.29 | 0.48 |
| 1:A:230:THR:HB | 1:A:302:GLN:OE1 | 2.14 | 0.47 |
| 1:C:179:ARG:HA | 1:C:183:ASP:OD1 | 2.13 | 0.47 |
| 1:D:78:LYS:O | 1:D:80:ILE:HD12 | 2.14 | 0.47 |
| 1:D:59:LEU:HB3 | 1:D:172:GLU:HG2 | 1.96 | 0.47 |
| 1:C:172:GLU:HB3 | 1:C:173:PRO:HD3 | 1.96 | 0.47 |
| 1:D:253:GLU:HA | 1:D:256:ASP:HB2 | 1.95 | 0.47 |
| 2:R:27:C:H2' | 2:R:28:C:O4' | 2.13 | 0.47 |
| 1:E:409:GLU:HG3 | 1:E:414:LYS:HD3 | 1.96 | 0.47 |
| 1:E:141:LEU:HD22 | 1:E:182:PHE:CE1 | 2.49 | 0.47 |
| 1:C:141:LEU:HD22 | 1:C:182:PHE:CD1 | 2.49 | 0.47 |
| 1:A:147:THR:CG2 | 1:A:152:TYR:HB3 | 2.44 | 0.47 |
| 1:B:43:ASN:OD1 | 1:B:112:ALA:HB3 | 2.15 | 0.47 |
| 1:A:46:LYS:HD3 | 1:A:46:LYS:N | 2.27 | 0.47 |
| 1:B:295:PRO:HB2 | 1:B:322:ILE:HG21 | 1.96 | 0.47 |
| 1:B:412:ILE:C | 1:B:412:ILE:HD12 | 2.34 | 0.47 |
| 1:D:36:LYS:HG3 | 1:D:93:ILE:HD11 | 1.96 | 0.47 |
| 1:E:144:VAL:O | 1:E:147:THR:HG22 | 2.14 | 0.47 |
| 1:C:317:ARG:CZ | 2:R:13:C:O2' | 2.62 | 0.47 |
| 1:D:153:ARG:CZ | 1:D:176:PRO:HA | 2.44 | 0.47 |
| 1:A:59:LEU:HB3 | 1:A:172:GLU:HG2 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:136:LEU:HD23 | 1:A:136:LEU:O | 2.15 | 0.47 |
| 1:C:398:LYS:HG2 | 1:C:402:MET:CE | 2.43 | 0.47 |
| 1:A:70:ASN:H | 1:A:70:ASN:HD22 | 1.60 | 0.47 |
| 1:A:45:THR:H | 1:A:111:LYS:NZ | 2.12 | 0.47 |
| 1:E:398:LYS:HG2 | 1:E:402:MET:CE | 2.43 | 0.47 |
| 1:A:180:ASP:OD2 | 1:A:180:ASP:O | 2.32 | 0.47 |
| 1:D:385:GLN:O | 1:D:386:ASN:HB2 | 2.14 | 0.47 |
| 1:A:409:GLU:HG3 | 1:A:414:LYS:HD3 | 1.96 | 0.47 |
| 1:E:163:GLN:C | 1:E:165:LYS:N | 2.67 | 0.47 |
| 1:A:141:LEU:HD22 | 1:A:182:PHE:CE1 | 2.50 | 0.47 |
| 1:D:354:LYS:CE | 1:D:356:THR:HA | 2.34 | 0.47 |
| 1:A:59:LEU:O | 1:A:61:SER:N | 2.47 | 0.47 |
| 1:E:54:TYR:OH | 1:E:120:GLY:N | 2.48 | 0.47 |
| 1:E:212:SER:HA | 2:R:45:C:C6 | 2.50 | 0.47 |
| 1:A:36:LYS:HG3 | 1:A:93:ILE:HD11 | 1.97 | 0.47 |
| 1:B:150:PRO:N | 1:B:152:TYR:CZ | 2.83 | 0.47 |
| 1:D:223:LYS:O | 1:D:224:ASP:HB2 | 2.15 | 0.47 |
| 1:C:105:PHE:C | 1:C:107:LEU:N | 2.67 | 0.47 |
| 1:B:171:PHE:CD2 | 1:B:172:GLU:N | 2.82 | 0.47 |
| 1:C:409:GLU:HG3 | 1:C:414:LYS:HD3 | 1.95 | 0.47 |
| 1:A:8:ILE:O | 1:A:8:ILE:HG13 | 2.15 | 0.47 |
| 1:E:177:GLU:HG2 | 1:E:178:GLY:H | 1.80 | 0.47 |
| 1:E:181:ILE:HB | 1:E:182:PHE:CD2 | 2.50 | 0.47 |
| 1:D:177:GLU:HG2 | 1:D:178:GLY:N | 2.30 | 0.47 |
| 1:A:149:MET:O | 1:A:152:TYR:CG | 2.68 | 0.47 |
| 1:A:149:MET:C | 1:A:152:TYR:CZ | 2.88 | 0.47 |
| 1:A:68:HIS:CE1 | 1:A:117:LEU:HG | 2.48 | 0.47 |
| 1:C:376:VAL:HG13 | 1:D:354:LYS:CA | 2.43 | 0.47 |
| 1:C:78:LYS:O | 1:C:80:ILE:HD12 | 2.14 | 0.47 |
| 1:C:78:LYS:O | 1:C:80:ILE:N | 2.47 | 0.47 |
| 1:C:43:ASN:OD1 | 1:C:112:ALA:HB3 | 2.15 | 0.47 |
| 1:C:122:SER:O | 1:C:123:ASP:HB2 | 2.14 | 0.47 |
| 1:D:136:LEU:O | 1:D:136:LEU:HD23 | 2.15 | 0.47 |
| 1:B:382:PHE:HE1 | 1:B:393:MET:HE1 | 1.78 | 0.47 |
| 1:A:328:THR:HG21 | 1:A:415:TYR:OH | 2.15 | 0.47 |
| 1:C:149:MET:C | 1:C:151:GLU:N | 2.63 | 0.47 |
| 1:A:29:ALA:C | 1:A:31:TYR:H | 2.13 | 0.47 |
| 1:A:89:SER:O | 1:A:90:SER:CB | 2.63 | 0.47 |
| 1:A:79:ASP:HB2 | 1:A:81:ARG:NE | 2.30 | 0.47 |
| 1:E:215:TYR:C | 1:E:215:TYR:CD2 | 2.87 | 0.47 |
| 1:E:55:VAL:HG12 | 1:E:64:VAL:HG21 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:163:GLN:O | 1:E:165:LYS:N | 2.48 | 0.47 |
| 2:R:21:C:C6 | 2:R:21:C:H5" | 2.39 | 0.47 |
| 1:D:55:VAL:HG12 | 1:D:64:VAL:HG21 | 1.97 | 0.47 |
| 1:D:147:THR:HG21 | 1:D:152:TYR:HA | 1.96 | 0.47 |
| 1:C:148:GLN:O | 1:C:152:TYR:CE2 | 2.68 | 0.47 |
| 1:D:364:LEU:HB3 | 1:D:368:ALA:CB | 2.45 | 0.47 |
| 1:E:68:HIS:CE1 | 1:E:117:LEU:HG | 2.49 | 0.47 |
| 1:B:38:ILE:HD11 | 1:B:107:LEU:O | 2.14 | 0.47 |
| 1:E:41:TYR:CE1 | 1:E:110:LEU:HD12 | 2.44 | 0.47 |
| 1:C:253:GLU:HA | 1:C:256:ASP:HB2 | 1.97 | 0.47 |
| 1:A:223:LYS:O | 1:A:224:ASP:HB2 | 2.14 | 0.47 |
| 1:E:28:PRO:O | 1:E:31:TYR:HB3 | 2.15 | 0.46 |
| 1:B:86:LYS:HB3 | 1:B:87:ASP:H | 1.56 | 0.46 |
| 1:B:81:ARG:HB2 | 1:B:208:HIS:NE2 | 2.29 | 0.46 |
| 1:B:208:HIS:CE1 | 1:B:210:CYS:HB2 | 2.50 | 0.46 |
| 1:E:293:LYS:C | 1:E:295:PRO:HD3 | 2.36 | 0.46 |
| 1:E:385:GLN:O | 1:E:386:ASN:HB2 | 2.15 | 0.46 |
| 1:D:293:LYS:C | 1:D:295:PRO:HD3 | 2.35 | 0.46 |
| 1:C:196:ALA:HB3 | 1:C:281:PHE:CE1 | 2.51 | 0.46 |
| 1:E:136:LEU:O | 1:E:136:LEU:HD23 | 2.16 | 0.46 |
| 1:E:179:ARG:HA | 1:E:183:ASP:OD1 | 2.15 | 0.46 |
| 1:A:18:LEU:HD12 | 1:B:232:GLY:CA | 2.45 | 0.46 |
| 1:B:283:LEU:HD23 | 1:B:283:LEU:N | 2.29 | 0.46 |
| 1:C:153:ARG:NH1 | 1:C:176:PRO:O | 2.44 | 0.46 |
| 1:E:72:TYR:CD2 | 1:E:72:TYR:C | 2.86 | 0.46 |
| 1:B:356:THR:CG2 | 1:B:357:PRO:HD3 | 2.31 | 0.46 |
| 1:E:107:LEU:HD23 | 1:E:274:TYR:HE2 | 1.81 | 0.46 |
| 1:B:172:GLU:HB3 | 1:B:173:PRO:CD | 2.45 | 0.46 |
| 1:B:59:LEU:HB3 | 1:B:172:GLU:HG2 | 1.97 | 0.46 |
| 1:B:293:LYS:C | 1:B:295:PRO:HD3 | 2.36 | 0.46 |
| 1:B:70:ASN:H | 1:B:70:ASN:HD22 | 1.60 | 0.46 |
| 1:D:151:GLU:HG2 | 1:D:155:LYS:HD3 | 1.98 | 0.46 |
| 1:A:179:ARG:HA | 1:A:183:ASP:OD1 | 2.15 | 0.46 |
| 1:E:317:ARG:HG3 | 2:R:40:C:C2 | 2.49 | 0.46 |
| 1:A:167:ILE:O | 1:A:168:ASN:HB2 | 2.16 | 0.46 |
| 1:C:14:ILE:CD1 | 1:D:259:VAL:HA | 2.44 | 0.46 |
| 1:A:81:ARG:CD | 1:A:208:HIS:HE2 | 2.28 | 0.46 |
| 1:E:283:LEU:N | 1:E:283:LEU:HD23 | 2.30 | 0.46 |
| 1:E:151:GLU:HA | 1:E:154:LYS:HB3 | 1.98 | 0.46 |
| 1:C:147:THR:CG2 | 1:C:152:TYR:HB3 | 2.45 | 0.46 |
| 1:B:54:TYR:OH | 1:B:120:GLY:N | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:78:LYS:O | 1:D:80:ILE:N | 2.48 | 0.46 |
| 1:E:74:TYR:O | 1:E:78:LYS:HD3 | 2.16 | 0.46 |
| 1:B:81:ARG:CD | 1:B:208:HIS:HE2 | 2.29 | 0.46 |
| 1:A:200:MET:HB2 | 1:A:277:TYR:CE2 | 2.51 | 0.46 |
| 1:B:58:GLY:O | 1:B:63:ASN:O | 2.34 | 0.46 |
| 1:A:237:ILE:CD1 | 1:A:310:SER:HB2 | 2.45 | 0.46 |
| 1:B:230:THR:HB | 1:B:302:GLN:OE1 | 2.15 | 0.46 |
| 1:C:181:ILE:HB | 1:C:182:PHE:CD2 | 2.51 | 0.46 |
| 1:A:177:GLU:HG2 | 1:A:178:GLY:H | 1.80 | 0.46 |
| 1:D:240:MET:HB3 | 1:D:240:MET:HE3 | 1.81 | 0.46 |
| 1:D:365:THR:HG23 | 1:D:366:THR:H | 1.81 | 0.46 |
| 1:E:226:ALA:HB2 | 2:R:40:C:H5' | 1.98 | 0.46 |
| 1:A:72:TYR:CD2 | 1:A:72:TYR:C | 2.85 | 0.46 |
| 1:D:45:THR:O | 1:D:46:LYS:HD3 | 2.15 | 0.46 |
| 1:C:45:THR:O | 1:C:46:LYS:HD3 | 2.15 | 0.46 |
| 1:A:78:LYS:HE2 | 1:A:78:LYS:HB2 | 1.76 | 0.46 |
| 1:E:37:GLU:CB | 1:E:108:VAL:HG11 | 2.40 | 0.46 |
| 1:A:105:PHE:C | 1:A:107:LEU:N | 2.64 | 0.46 |
| 1:A:37:GLU:HB2 | 1:A:108:VAL:HG21 | 1.98 | 0.46 |
| 1:C:14:ILE:HD12 | 1:D:259:VAL:HG22 | 1.98 | 0.46 |
| 1:C:240:MET:HE3 | 1:C:244:ASP:CB | 2.46 | 0.46 |
| 1:A:153:ARG:CZ | 1:A:176:PRO:HA | 2.46 | 0.46 |
| 1:B:147:THR:CG2 | 1:B:152:TYR:HB3 | 2.46 | 0.46 |
| 1:B:68:HIS:CE1 | 1:B:118:PRO:HD2 | 2.51 | 0.46 |
| 1:A:167:ILE:HG22 | 1:A:169:GLU:CD | 2.36 | 0.46 |
| 1:C:107:LEU:HD23 | 1:C:274:TYR:HE2 | 1.80 | 0.46 |
| 1:A:253:GLU:N | 1:A:253:GLU:OE2 | 2.44 | 0.46 |
| 1:C:41:TYR:CE1 | 1:C:110:LEU:HD12 | 2.47 | 0.46 |
| 1:C:226:ALA:HB3 | 1:C:291:SER:HB3 | 1.98 | 0.46 |
| 1:B:149:MET:C | 1:B:152:TYR:CZ | 2.89 | 0.46 |
| 1:D:81:ARG:HB2 | 1:D:208:HIS:NE2 | 2.31 | 0.46 |
| 1:E:148:GLN:O | 1:E:152:TYR:CE2 | 2.68 | 0.46 |
| 2:R:9:C:C6 | 2:R:10:C:C5 | 3.04 | 0.46 |
| 1:D:144:VAL:O | 1:D:147:THR:HG22 | 2.15 | 0.46 |
| 1:A:65:SER:HB3 | 1:A:68:HIS:ND1 | 2.31 | 0.46 |
| 1:A:107:LEU:HD23 | 1:A:274:TYR:HE2 | 1.81 | 0.46 |
| 1:B:255:ALA:O | 1:B:256:ASP:C | 2.53 | 0.46 |
| 1:E:382:PHE:CD2 | 1:E:387:ARG:HA | 2.50 | 0.46 |
| 1:A:55:VAL:HG12 | 1:A:64:VAL:HG21 | 1.97 | 0.46 |
| 1:A:401:VAL:HG21 | 1:A:420:PHE:HB2 | 1.96 | 0.46 |
| 1:B:408:ARG:HD3 | 2:R:24:C:C4 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:147:THR:HG21 | 1:E:152:TYR:HA | 1.97 | 0.45 |
| 1:D:181:ILE:HB | 1:D:182:PHE:CD2 | 2.51 | 0.45 |
| 1:E:223:LYS:O | 1:E:224:ASP:HB2 | 2.16 | 0.45 |
| 1:B:54:TYR:CE1 | 1:B:122:SER:HB2 | 2.51 | 0.45 |
| 1:D:37:GLU:HB2 | 1:D:108:VAL:HG21 | 1.98 | 0.45 |
| 1:B:203:HIS:HD2 | 1:B:272:ASP:OD1 | 1.98 | 0.45 |
| 1:B:401:VAL:HG21 | 1:B:420:PHE:HB2 | 1.96 | 0.45 |
| 1:D:283:LEU:HD23 | 1:D:283:LEU:N | 2.30 | 0.45 |
| 1:C:177:GLU:HG2 | 1:C:178:GLY:H | 1.81 | 0.45 |
| 1:A:54:TYR:CD1 | 1:A:118:PRO:HB2 | 2.50 | 0.45 |
| 1:B:107:LEU:HD23 | 1:B:274:TYR:HE2 | 1.80 | 0.45 |
| 1:E:172:GLU:HB3 | 1:E:173:PRO:HD3 | 1.98 | 0.45 |
| 1:C:119:ASP:OD1 | 1:C:119:ASP:N | 2.50 | 0.45 |
| 1:E:167:ILE:HG22 | 1:E:168:ASN:H | 1.80 | 0.45 |
| 1:C:317:ARG:CD | 1:C:317:ARG:H | 2.30 | 0.45 |
| 1:B:151:GLU:HA | 1:B:154:LYS:HB3 | 1.99 | 0.45 |
| 1:D:226:ALA:HB2 | 2:R:4:C:O5' | 2.17 | 0.45 |
| 1:D:317:ARG:N | 1:D:317:ARG:CZ | 2.74 | 0.45 |
| 1:D:42:ILE:HD12 | 1:D:74:TYR:CB | 2.38 | 0.45 |
| 1:E:409:GLU:HA | 1:E:414:LYS:HD2 | 1.99 | 0.45 |
| 1:B:317:ARG:NH2 | 2:R:23:C:C5' | 2.59 | 0.45 |
| 1:B:153:ARG:NH1 | 1:B:176:PRO:O | 2.47 | 0.45 |
| 1:D:89:SER:O | 1:D:90:SER:CB | 2.64 | 0.45 |
| 1:C:81:ARG:CD | 1:C:208:HIS:HE2 | 2.29 | 0.45 |
| 1:C:70:ASN:H | 1:C:70:ASN:HD22 | 1.65 | 0.45 |
| 1:D:240:MET:HE3 | 1:D:244:ASP:CB | 2.47 | 0.45 |
| 1:D:409:GLU:HG3 | 1:D:414:LYS:HD3 | 1.97 | 0.45 |
| 1:E:328:THR:HG21 | 1:E:415:TYR:OH | 2.16 | 0.45 |
| 2:R:32:C:N4 | 2:R:34:C:C5 | 2.84 | 0.45 |
| 1:D:74:TYR:O | 1:D:78:LYS:HD3 | 2.16 | 0.45 |
| 1:B:385:GLN:HG2 | 1:B:390:THR:CG2 | 2.47 | 0.45 |
| 1:D:238:THR:C | 1:D:240:MET:H | 2.20 | 0.45 |
| 1:C:15:VAL:O | 1:C:17:LYS:HG2 | 2.17 | 0.45 |
| 1:A:283:LEU:N | 1:A:283:LEU:HD23 | 2.32 | 0.45 |
| 1:D:141:LEU:HD22 | 1:D:182:PHE:CD1 | 2.52 | 0.45 |
| 1:A:59:LEU:O | 1:A:61:SER:O | 2.34 | 0.45 |
| 1:D:172:GLU:HB3 | 1:D:173:PRO:HD3 | 1.98 | 0.45 |
| 1:E:27:TYR:HB3 | 1:E:266:GLN:HE22 | 1.82 | 0.45 |
| 1:E:55:VAL:O | 1:E:56:TYR:C | 2.55 | 0.45 |
| 1:C:3:VAL:O | 1:C:4:THR:HB | 2.15 | 0.45 |
| 1:C:150:PRO:HD3 | 1:C:152:TYR:OH | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:253:GLU:HA | 1:E:256:ASP:HB2 | 1.98 | 0.45 |
| 1:B:41:TYR:CE1 | 1:B:110:LEU:HD12 | 2.50 | 0.45 |
| 1:D:54:TYR:CD1 | 1:D:118:PRO:HB2 | 2.52 | 0.45 |
| 1:C:38:ILE:O | 1:C:108:VAL:HB | 2.16 | 0.45 |
| 1:E:81:ARG:CD | 1:E:208:HIS:HE2 | 2.29 | 0.45 |
| 1:B:79:ASP:HB2 | 1:B:81:ARG:NE | 2.32 | 0.45 |
| 1:A:313:ALA:O | 1:A:412:ILE:HD11 | 2.17 | 0.45 |
| 1:B:8:ILE:O | 1:B:8:ILE:HG13 | 2.17 | 0.45 |
| 1:D:196:ALA:HB3 | 1:D:281:PHE:CE1 | 2.52 | 0.45 |
| 1:E:153:ARG:CZ | 1:E:176:PRO:HA | 2.47 | 0.45 |
| 1:C:184:VAL:HG11 | 1:D:166:MET:N | 2.32 | 0.45 |
| 1:E:105:PHE:C | 1:E:107:LEU:N | 2.67 | 0.45 |
| 1:A:163:GLN:CD | 1:A:163:GLN:N | 2.71 | 0.45 |
| 1:B:91:PHE:CE2 | 1:B:267:GLU:HG3 | 2.52 | 0.45 |
| 1:A:22:GLU:HB3 | 1:B:206:LYS:NZ | 2.32 | 0.45 |
| 1:A:382:PHE:CD2 | 1:A:387:ARG:HA | 2.52 | 0.45 |
| 1:C:275:MET:HB3 | 1:C:276:PRO:HD3 | 1.99 | 0.45 |
| 1:A:238:THR:C | 1:A:240:MET:H | 2.20 | 0.45 |
| 1:E:150:PRO:HD3 | 1:E:152:TYR:OH | 2.17 | 0.45 |
| 1:A:181:ILE:HB | 1:A:182:PHE:CD2 | 2.52 | 0.45 |
| 1:A:167:ILE:CG2 | 1:A:169:GLU:HG2 | 2.43 | 0.45 |
| 1:E:259:VAL:O | 1:E:260:GLN:C | 2.54 | 0.45 |
| 1:A:241:SER:O | 1:A:245:VAL:HG23 | 2.17 | 0.45 |
| 1:A:275:MET:HB3 | 1:A:276:PRO:HD3 | 1.98 | 0.45 |
| 1:E:218:ILE:C | 1:E:220:SER:H | 2.20 | 0.45 |
| 1:D:215:TYR:C | 1:D:215:TYR:CD2 | 2.90 | 0.44 |
| 1:A:144:VAL:O | 1:A:147:THR:HG22 | 2.17 | 0.44 |
| 1:B:165:LYS:O | 1:B:167:ILE:CD1 | 2.65 | 0.44 |
| 1:E:401:VAL:HG21 | 1:E:420:PHE:HB2 | 1.98 | 0.44 |
| 1:E:168:ASN:O | 1:E:169:GLU:HB2 | 2.17 | 0.44 |
| 1:C:144:VAL:O | 1:C:147:THR:HG22 | 2.17 | 0.44 |
| 1:E:366:THR:C | 1:E:368:ALA:H | 2.21 | 0.44 |
| 1:E:31:TYR:C | 1:E:33:ARG:H | 2.20 | 0.44 |
| 1:A:28:PRO:O | 1:A:29:ALA:C | 2.55 | 0.44 |
| 1:D:397:ALA:O | 1:D:401:VAL:HG22 | 2.17 | 0.44 |
| 1:A:184:VAL:HG13 | 1:B:165:LYS:HG3 | 1.99 | 0.44 |
| 1:E:29:ALA:HB2 | 1:E:91:PHE:HE2 | 1.81 | 0.44 |
| 1:B:218:ILE:C | 1:B:220:SER:H | 2.21 | 0.44 |
| 1:E:149:MET:HG3 | 2:R:42:C:C6 | 2.53 | 0.44 |
| 1:B:147:THR:HG21 | 1:B:152:TYR:HA | 1.98 | 0.44 |
| 1:E:317:ARG:HH21 | 2:R:41:C:H5' | 1.73 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:45:THR:O | 1:A:46:LYS:HD3 | 2.18 | 0.44 |
| 1:E:364:LEU:O | 1:E:365:THR:C | 2.56 | 0.44 |
| 1:C:208:HIS:CE1 | 1:C:210:CYS:HB2 | 2.52 | 0.44 |
| 1:C:81:ARG:HB2 | 1:C:208:HIS:NE2 | 2.32 | 0.44 |
| 1:B:275:MET:HB3 | 1:B:276:PRO:HD3 | 1.99 | 0.44 |
| 1:E:46:LYS:HA | 1:E:46:LYS:HD3 | 1.70 | 0.44 |
| 1:A:208:HIS:CE1 | 1:A:210:CYS:HB2 | 2.52 | 0.44 |
| 1:A:364:LEU:HD22 | 1:A:368:ALA:HB2 | 2.00 | 0.44 |
| 1:C:397:ALA:O | 1:C:401:VAL:HG22 | 2.17 | 0.44 |
| 1:C:218:ILE:C | 1:C:220:SER:H | 2.20 | 0.44 |
| 1:B:409:GLU:HG3 | 1:B:414:LYS:HD3 | 1.99 | 0.44 |
| 1:A:147:THR:HG21 | 1:A:152:TYR:HA | 1.99 | 0.44 |
| 1:A:376:VAL:HG13 | 1:B:354:LYS:CB | 2.45 | 0.44 |
| 1:C:354:LYS:CE | 1:C:356:THR:HA | 2.38 | 0.44 |
| 1:A:172:GLU:HB3 | 1:A:173:PRO:HD3 | 1.99 | 0.44 |
| 1:E:45:THR:O | 1:E:46:LYS:HD3 | 2.18 | 0.44 |
| 1:C:54:TYR:OH | 1:C:120:GLY:N | 2.50 | 0.44 |
| 1:B:103:GLY:N | 1:B:106:ASP:OD2 | 2.48 | 0.44 |
| 1:D:91:PHE:CE2 | 1:D:267:GLU:HG3 | 2.51 | 0.44 |
| 1:D:14:ILE:HG23 | 1:D:16:PRO:HD3 | 1.99 | 0.44 |
| 1:B:328:THR:HG21 | 1:B:415:TYR:OH | 2.17 | 0.44 |
| 1:B:177:GLU:HG2 | 1:B:178:GLY:H | 1.81 | 0.44 |
| 1:E:365:THR:HG23 | 1:E:366:THR:H | 1.83 | 0.44 |
| 1:C:249:ILE:HD13 | 1:C:254:VAL:HG12 | 1.99 | 0.44 |
| 1:B:238:THR:C | 1:B:240:MET:H | 2.21 | 0.44 |
| 1:A:18:LEU:CD1 | 1:B:232:GLY:HA2 | 2.48 | 0.44 |
| 1:C:55:VAL:HG12 | 1:C:64:VAL:HG21 | 1.99 | 0.44 |
| 1:D:181:ILE:CD1 | 1:D:181:ILE:H | 2.26 | 0.44 |
| 1:A:150:PRO:N | 1:A:152:TYR:CZ | 2.86 | 0.44 |
| 1:B:153:ARG:HH12 | 1:B:177:GLU:HB2 | 1.83 | 0.44 |
| 1:D:113:LEU:N | 1:D:113:LEU:HD23 | 2.33 | 0.44 |
| 1:C:90:SER:O | 1:C:91:PHE:HB2 | 2.18 | 0.44 |
| 1:C:253:GLU:N | 1:C:253:GLU:OE2 | 2.44 | 0.44 |
| 1:E:196:ALA:HB3 | 1:E:281:PHE:CE1 | 2.53 | 0.44 |
| 1:E:275:MET:SD | 1:E:275:MET:C | 2.96 | 0.44 |
| 2:R:9:C:H2' | 2:R:10:C:O4' | 2.17 | 0.44 |
| 1:C:151:GLU:HA | 1:C:154:LYS:HB3 | 2.00 | 0.44 |
| 1:A:151:GLU:HA | 1:A:154:LYS:HB3 | 2.00 | 0.44 |
| 1:B:144:VAL:O | 1:B:147:THR:HG22 | 2.17 | 0.44 |
| 1:B:181:ILE:HB | 1:B:182:PHE:CD2 | 2.53 | 0.44 |
| 1:C:165:LYS:HZ3 | 1:C:165:LYS:CB | 2.30 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:7:ARG:NH2 | 1:D:256:ASP:OD2 | 2.51 | 0.44 |
| 1:E:79:ASP:HB2 | 1:E:81:ARG:NE | 2.32 | 0.44 |
| 1:E:81:ARG:HB2 | 1:E:208:HIS:NE2 | 2.33 | 0.44 |
| 1:D:107:LEU:HD23 | 1:D:274:TYR:HE2 | 1.83 | 0.44 |
| 1:E:149:MET:C | 1:E:152:TYR:CE2 | 2.91 | 0.43 |
| 1:B:141:LEU:HD22 | 1:B:182:PHE:CE1 | 2.53 | 0.43 |
| 1:E:68:HIS:CE1 | 1:E:118:PRO:HD2 | 2.53 | 0.43 |
| 1:D:54:TYR:CE1 | 1:D:122:SER:HB2 | 2.53 | 0.43 |
| 1:D:54:TYR:OH | 1:D:120:GLY:N | 2.50 | 0.43 |
| 1:A:78:LYS:O | 1:A:80:ILE:HD12 | 2.18 | 0.43 |
| 1:B:342:ALA:HB1 | 1:B:344:LEU:HD23 | 1.99 | 0.43 |
| 1:E:238:THR:C | 1:E:240:MET:H | 2.21 | 0.43 |
| 1:E:151:GLU:HG2 | 1:E:155:LYS:HD3 | 1.99 | 0.43 |
| 1:E:141:LEU:HD22 | 1:E:182:PHE:CD1 | 2.53 | 0.43 |
| 1:D:46:LYS:N | 1:D:46:LYS:HD3 | 2.24 | 0.43 |
| 1:B:349:CYS:SG | 1:E:8:ILE:CG2 | 3.02 | 0.43 |
| 1:A:409:GLU:HA | 1:A:414:LYS:HD2 | 2.00 | 0.43 |
| 1:E:149:MET:O | 1:E:152:TYR:CD2 | 2.71 | 0.43 |
| 1:E:410:LYS:HZ1 | 2:R:40:C:H42 | 1.65 | 0.43 |
| 2:R:39:C:H5' | 2:R:40:C:OP2 | 2.19 | 0.43 |
| 1:B:65:SER:HB3 | 1:B:68:HIS:ND1 | 2.33 | 0.43 |
| 1:D:43:ASN:OD1 | 1:D:112:ALA:HB3 | 2.18 | 0.43 |
| 1:B:29:ALA:C | 1:B:31:TYR:N | 2.72 | 0.43 |
| 1:C:228:LEU:O | 1:C:228:LEU:HD22 | 2.18 | 0.43 |
| 1:D:323:GLU:O | 1:D:327:LEU:HD22 | 2.18 | 0.43 |
| 1:C:18:LEU:CD1 | 1:D:232:GLY:HA2 | 2.49 | 0.43 |
| 1:C:215:TYR:CD2 | 1:C:215:TYR:C | 2.91 | 0.43 |
| 1:D:153:ARG:NH2 | 1:D:176:PRO:HA | 2.33 | 0.43 |
| 2:R:40:C:C2' | 2:R:40:C:O2 | 2.66 | 0.43 |
| 1:E:199:ASP:OD1 | 1:E:217:THR:HG23 | 2.18 | 0.43 |
| 1:B:303:LEU:CD2 | 1:B:328:THR:HA | 2.48 | 0.43 |
| 1:E:342:ALA:HB1 | 1:E:344:LEU:HD23 | 2.00 | 0.43 |
| 1:B:170:GLN:HB3 | 1:B:170:GLN:HE21 | 1.59 | 0.43 |
| 1:A:168:ASN:C | 1:A:169:GLU:OE2 | 2.57 | 0.43 |
| 1:B:376:VAL:HG13 | 1:C:354:LYS:CA | 2.48 | 0.43 |
| 1:B:383:GLU:CG | 1:C:354:LYS:HE2 | 2.46 | 0.43 |
| 1:B:45:THR:O | 1:B:46:LYS:HD3 | 2.18 | 0.43 |
| 1:D:123:ASP:C | 1:D:125:SER:H | 2.22 | 0.43 |
| 1:D:398:LYS:HG2 | 1:D:402:MET:CE | 2.47 | 0.43 |
| 1:B:316:ALA:HA | 1:B:317:ARG:CZ | 2.47 | 0.43 |
| 2:R:9:C:C5 | 2:R:10:C:C5 | 3.06 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:149:MET:O | 1:D:152:TYR:CD2 | 2.72 | 0.43 |
| 1:D:151:GLU:HA | 1:D:154:LYS:HB3 | 2.01 | 0.43 |
| 1:C:149:MET:C | 1:C:152:TYR:CE2 | 2.91 | 0.43 |
| 1:B:134:LEU:N | 1:B:135:PRO:CD | 2.82 | 0.43 |
| 1:B:78:LYS:O | 1:B:80:ILE:N | 2.52 | 0.43 |
| 1:A:343:ASP:HB2 | 1:A:344:LEU:H | 1.68 | 0.43 |
| 1:C:247:THR:HA | 1:D:348:PHE:HB2 | 2.01 | 0.43 |
| 1:D:4:THR:HG23 | 1:D:4:THR:O | 2.18 | 0.43 |
| 1:C:230:THR:HB | 1:C:302:GLN:OE1 | 2.19 | 0.43 |
| 1:B:149:MET:O | 1:B:152:TYR:CG | 2.71 | 0.43 |
| 1:A:167:ILE:O | 1:A:169:GLU:OE1 | 2.37 | 0.43 |
| 1:C:136:LEU:CD2 | 1:C:163:GLN:HE21 | 2.25 | 0.43 |
| 1:B:171:PHE:CZ | 1:B:173:PRO:CG | 3.00 | 0.43 |
| 1:D:81:ARG:CD | 1:D:208:HIS:HE2 | 2.32 | 0.43 |
| 1:D:105:PHE:C | 1:D:107:LEU:N | 2.70 | 0.43 |
| 1:D:164:CYS:HA | 1:D:168:ASN:HA | 2.00 | 0.43 |
| 1:A:364:LEU:O | 1:A:366:THR:N | 2.52 | 0.43 |
| 1:D:149:MET:C | 1:D:152:TYR:CE2 | 2.92 | 0.43 |
| 1:E:230:THR:HB | 1:E:302:GLN:OE1 | 2.18 | 0.43 |
| 1:B:19:PRO:CG | 1:C:228:LEU:CD1 | 2.96 | 0.43 |
| 1:D:233:HIS:HB2 | 1:D:312:ARG:NH1 | 2.33 | 0.43 |
| 1:A:54:TYR:OH | 1:A:120:GLY:N | 2.52 | 0.43 |
| 1:C:54:TYR:CE1 | 1:C:122:SER:HB2 | 2.53 | 0.43 |
| 1:B:136:LEU:O | 1:B:136:LEU:HD23 | 2.19 | 0.43 |
| 1:B:163:GLN:N | 1:B:163:GLN:CD | 2.73 | 0.43 |
| 1:B:228:LEU:HD22 | 1:B:228:LEU:O | 2.19 | 0.43 |
| 1:C:79:ASP:HB2 | 1:C:81:ARG:NE | 2.34 | 0.43 |
| 1:B:366:THR:C | 1:B:368:ALA:H | 2.21 | 0.43 |
| 1:D:342:ALA:HB1 | 1:D:344:LEU:HD23 | 2.00 | 0.43 |
| 2:R:10:C:C5' | 2:R:11:C:OP2 | 2.67 | 0.43 |
| 1:D:150:PRO:HD3 | 1:D:152:TYR:OH | 2.19 | 0.43 |
| 1:A:112:ALA:HB1 | 1:A:113:LEU:HD23 | 1.99 | 0.43 |
| 1:B:172:GLU:HB3 | 1:B:173:PRO:HD3 | 2.00 | 0.43 |
| 1:E:165:LYS:HZ3 | 1:E:165:LYS:HB2 | 1.83 | 0.42 |
| 1:D:81:ARG:HD2 | 1:D:208:HIS:NE2 | 2.34 | 0.42 |
| 1:E:87:ASP:O | 1:E:88:TRP:HB2 | 2.18 | 0.42 |
| 1:A:385:GLN:HG2 | 1:A:390:THR:CG2 | 2.48 | 0.42 |
| 1:D:409:GLU:HA | 1:D:414:LYS:HD2 | 2.01 | 0.42 |
| 1:D:421:ASP:O | 1:D:422:LYS:HB3 | 2.19 | 0.42 |
| 1:E:90:SER:O | 1:E:91:PHE:HB2 | 2.18 | 0.42 |
| 1:A:91:PHE:CE2 | 1:A:267:GLU:HG3 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:255:ALA:O | 1:D:259:VAL:HG23 | 2.20 | 0.42 |
| 1:A:402:MET:HE2 | 1:A:402:MET:HB3 | 1.90 | 0.42 |
| 1:A:240:MET:HE3 | 1:A:244:ASP:HB3 | 2.02 | 0.42 |
| 1:D:218:ILE:C | 1:D:220:SER:H | 2.23 | 0.42 |
| 1:D:356:THR:CG2 | 1:D:357:PRO:HD3 | 2.35 | 0.42 |
| 1:C:241:SER:OG | 1:C:243:GLU:HG2 | 2.19 | 0.42 |
| 1:C:38:ILE:CD1 | 1:C:107:LEU:O | 2.67 | 0.42 |
| 1:B:214:ARG:O | 1:B:215:TYR:C | 2.55 | 0.42 |
| 1:E:89:SER:O | 1:E:90:SER:CB | 2.64 | 0.42 |
| 1:D:412:ILE:HD12 | 1:D:413:GLY:N | 2.34 | 0.42 |
| 1:A:55:VAL:HG12 | 1:A:64:VAL:CG2 | 2.49 | 0.42 |
| 1:D:202:PHE:CG | 1:D:211:ALA:HA | 2.54 | 0.42 |
| 1:B:55:VAL:HG12 | 1:B:64:VAL:HG21 | 2.00 | 0.42 |
| 1:B:4:THR:O | 1:B:4:THR:HG23 | 2.20 | 0.42 |
| 1:C:147:THR:HG21 | 1:C:152:TYR:HA | 2.00 | 0.42 |
| 1:B:57:GLN:HE21 | 1:B:60:LYS:NZ | 2.18 | 0.42 |
| 1:A:68:HIS:CE1 | 1:A:118:PRO:HD2 | 2.55 | 0.42 |
| 1:A:54:TYR:CE1 | 1:A:122:SER:HB2 | 2.54 | 0.42 |
| 1:E:356:THR:CG2 | 1:E:357:PRO:HD3 | 2.34 | 0.42 |
| 1:D:79:ASP:HB2 | 1:D:81:ARG:NE | 2.34 | 0.42 |
| 1:E:163:GLN:CD | 1:E:163:GLN:N | 2.73 | 0.42 |
| 1:C:112:ALA:HB1 | 1:C:113:LEU:HD23 | 2.01 | 0.42 |
| 1:A:78:LYS:O | 1:A:80:ILE:N | 2.53 | 0.42 |
| 1:A:103:GLY:N | 1:A:106:ASP:OD2 | 2.49 | 0.42 |
| 1:C:105:PHE:O | 1:C:107:LEU:N | 2.52 | 0.42 |
| 1:C:255:ALA:O | 1:C:256:ASP:C | 2.56 | 0.42 |
| 1:C:8:ILE:O | 1:C:8:ILE:HG13 | 2.19 | 0.42 |
| 1:E:54:TYR:CE1 | 1:E:122:SER:HB2 | 2.54 | 0.42 |
| 1:D:226:ALA:HB3 | 1:D:291:SER:HB3 | 2.02 | 0.42 |
| 1:D:224:ASP:HA | 2:R:4:C:OP1 | 2.19 | 0.42 |
| 1:C:170:GLN:HB3 | 1:C:171:PHE:H | 1.42 | 0.42 |
| 1:D:55:VAL:HG12 | 1:D:64:VAL:CG2 | 2.50 | 0.42 |
| 1:B:196:ALA:HB3 | 1:B:281:PHE:CE1 | 2.55 | 0.42 |
| 1:D:366:THR:C | 1:D:368:ALA:H | 2.22 | 0.42 |
| 1:A:380:GLY:CA | 1:B:354:LYS:HZ3 | 2.27 | 0.42 |
| 1:D:90:SER:O | 1:D:91:PHE:HB2 | 2.20 | 0.42 |
| 1:D:228:LEU:O | 1:D:228:LEU:HD22 | 2.19 | 0.42 |
| 1:A:31:TYR:CD1 | 1:A:32:PHE:N | 2.88 | 0.42 |
| 1:D:208:HIS:CE1 | 1:D:210:CYS:HB2 | 2.54 | 0.42 |
| 1:A:295:PRO:HB2 | 1:A:322:ILE:HG21 | 2.02 | 0.42 |
| 1:C:409:GLU:HA | 1:C:414:LYS:HD2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:263:LEU:HD12 | 1:D:263:LEU:HA | 1.91 | 0.42 |
| 1:E:54:TYR:CD1 | 1:E:118:PRO:HB2 | 2.52 | 0.42 |
| 1:A:74:TYR:O | 1:A:78:LYS:HD3 | 2.19 | 0.42 |
| 1:C:255:ALA:O | 1:C:259:VAL:HG23 | 2.20 | 0.42 |
| 1:B:66:ILE:HD13 | 1:B:185:TRP:CD1 | 2.54 | 0.42 |
| 1:A:81:ARG:HB2 | 1:A:208:HIS:NE2 | 2.34 | 0.42 |
| 1:B:369:PRO:HB3 | 1:B:381:TRP:CZ2 | 2.55 | 0.42 |
| 1:D:399:ARG:HB3 | 1:D:399:ARG:NH1 | 2.35 | 0.42 |
| 1:E:119:ASP:OD1 | 1:E:119:ASP:N | 2.53 | 0.42 |
| 1:D:65:SER:HB3 | 1:D:68:HIS:ND1 | 2.34 | 0.42 |
| 1:C:103:GLY:N | 1:C:106:ASP:OD2 | 2.47 | 0.42 |
| 1:B:382:PHE:CD2 | 1:B:387:ARG:HA | 2.55 | 0.42 |
| 1:D:180:ASP:O | 1:D:180:ASP:OD2 | 2.38 | 0.42 |
| 1:B:55:VAL:O | 1:B:56:TYR:C | 2.57 | 0.42 |
| 1:B:231:PHE:HB2 | 1:B:297:PHE:CZ | 2.54 | 0.42 |
| 1:E:399:ARG:NH1 | 1:E:399:ARG:HB3 | 2.35 | 0.42 |
| 1:E:167:ILE:O | 1:E:168:ASN:HB2 | 2.18 | 0.42 |
| 1:B:153:ARG:CZ | 1:B:176:PRO:HA | 2.50 | 0.42 |
| 1:C:163:GLN:N | 1:C:163:GLN:CD | 2.73 | 0.42 |
| 1:D:253:GLU:N | 1:D:253:GLU:CD | 2.71 | 0.42 |
| 1:B:18:LEU:HD11 | 1:C:232:GLY:HA2 | 2.01 | 0.42 |
| 1:B:237:ILE:CD1 | 1:B:310:SER:HB2 | 2.50 | 0.42 |
| 1:A:317:ARG:CD | 2:R:31:C:H2' | 2.48 | 0.41 |
| 1:C:65:SER:HB3 | 1:C:68:HIS:ND1 | 2.34 | 0.41 |
| 1:D:313:ALA:O | 1:D:412:ILE:HD11 | 2.20 | 0.41 |
| 1:E:397:ALA:O | 1:E:401:VAL:HG22 | 2.20 | 0.41 |
| 1:E:249:ILE:HD13 | 1:E:254:VAL:HG12 | 2.02 | 0.41 |
| 1:C:298:HIS:NE2 | 1:C:317:ARG:NH1 | 2.66 | 0.41 |
| 1:C:42:ILE:O | 1:C:43:ASN:O | 2.38 | 0.41 |
| 1:B:74:TYR:O | 1:B:78:LYS:HD3 | 2.20 | 0.41 |
| 1:A:37:GLU:CB | 1:A:108:VAL:HG11 | 2.44 | 0.41 |
| 1:E:363:GLY:C | 1:E:365:THR:H | 2.23 | 0.41 |
| 1:D:255:ALA:O | 1:D:256:ASP:C | 2.56 | 0.41 |
| 1:E:385:GLN:HG2 | 1:E:390:THR:CG2 | 2.51 | 0.41 |
| 1:D:397:ALA:HB1 | 1:D:420:PHE:CG | 2.55 | 0.41 |
| 1:C:238:THR:O | 1:C:240:MET:N | 2.53 | 0.41 |
| 1:D:195:VAL:CG2 | 1:D:196:ALA:N | 2.82 | 0.41 |
| 1:E:190:ASN:O | 1:E:194:ILE:HG13 | 2.20 | 0.41 |
| 1:E:160:LEU:HA | 1:E:163:GLN:OE1 | 2.20 | 0.41 |
| 1:A:43:ASN:OD1 | 1:A:112:ALA:HB3 | 2.20 | 0.41 |
| 1:A:73:LEU:O | 1:A:74:TYR:C | 2.59 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:E:255:ALA:O | 1:E:256:ASP:C | 2.59 | 0.41 |
| 2:R:25:C:H2' | 2:R:26:C:H6 | 1.82 | 0.41 |
| 1:E:93:ILE:N | 1:E:93:ILE:HD12 | 2.35 | 0.41 |
| 1:E:369:PRO:HA | 1:E:370:PRO:HD3 | 1.81 | 0.41 |
| 1:C:18:LEU:HD12 | 1:D:232:GLY:CA | 2.50 | 0.41 |
| 1:C:149:MET:O | 1:C:152:TYR:CD2 | 2.74 | 0.41 |
| 1:A:356:THR:CG2 | 1:A:357:PRO:HD3 | 2.36 | 0.41 |
| 1:D:317:ARG:H | 1:D:317:ARG:CD | 2.34 | 0.41 |
| 1:B:158:ASP:C | 1:B:160:LEU:H | 2.24 | 0.41 |
| 1:B:105:PHE:O | 1:B:107:LEU:N | 2.51 | 0.41 |
| 1:B:38:ILE:O | 1:B:108:VAL:HB | 2.21 | 0.41 |
| 1:B:90:SER:O | 1:B:91:PHE:HB2 | 2.20 | 0.41 |
| 1:E:4:THR:HG23 | 1:E:4:THR:O | 2.21 | 0.41 |
| 1:C:249:ILE:HD12 | 1:D:348:PHE:HE1 | 1.85 | 0.41 |
| 1:C:55:VAL:O | 1:C:56:TYR:C | 2.58 | 0.41 |
| 2:R:1:C:H2' | 2:R:2:C:O4' | 2.20 | 0.41 |
| 1:D:275:MET:HB3 | 1:D:276:PRO:HD3 | 2.03 | 0.41 |
| 1:B:181:ILE:H | 1:B:181:ILE:CD1 | 2.24 | 0.41 |
| 1:B:263:LEU:HD12 | 1:B:263:LEU:HA | 1.88 | 0.41 |
| 1:C:382:PHE:O | 1:C:383:GLU:C | 2.59 | 0.41 |
| 1:E:38:ILE:CD1 | 1:E:107:LEU:O | 2.69 | 0.41 |
| 1:B:160:LEU:HA | 1:B:163:GLN:OE1 | 2.21 | 0.41 |
| 1:D:29:ALA:C | 1:D:31:TYR:N | 2.71 | 0.41 |
| 1:B:81:ARG:HD2 | 1:B:208:HIS:NE2 | 2.33 | 0.41 |
| 1:A:369:PRO:HA | 1:A:370:PRO:HD3 | 1.80 | 0.41 |
| 1:D:88:TRP:CD2 | 1:D:204:MET:HE3 | 2.56 | 0.41 |
| 1:A:195:VAL:CG2 | 1:A:196:ALA:N | 2.83 | 0.41 |
| 1:C:200:MET:HB2 | 1:C:277:TYR:CE2 | 2.56 | 0.41 |
| 1:D:153:ARG:HH12 | 1:D:177:GLU:HB2 | 1.86 | 0.41 |
| 1:A:151:GLU:HG2 | 1:A:155:LYS:HD3 | 2.02 | 0.41 |
| 1:A:160:LEU:HA | 1:A:163:GLN:OE1 | 2.20 | 0.41 |
| 1:D:398:LYS:O | 1:D:402:MET:HG2 | 2.20 | 0.41 |
| 1:B:397:ALA:HB1 | 1:B:420:PHE:CG | 2.55 | 0.41 |
| 1:B:195:VAL:CG2 | 1:B:196:ALA:N | 2.83 | 0.41 |
| 1:D:248:TRP:O | 1:D:250:LEU:HG | 2.20 | 0.41 |
| 1:D:177:GLU:HG2 | 1:D:178:GLY:H | 1.84 | 0.41 |
| 1:C:68:HIS:CE1 | 1:C:118:PRO:HD2 | 2.56 | 0.41 |
| 1:E:78:LYS:HB2 | 1:E:78:LYS:HE2 | 1.73 | 0.41 |
| 1:C:160:LEU:HA | 1:C:163:GLN:OE1 | 2.21 | 0.41 |
| 1:B:31:TYR:C | 1:B:33:ARG:N | 2.74 | 0.41 |
| 1:E:195:VAL:CG2 | 1:E:196:ALA:N | 2.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:158:ASP:C | 1:D:160:LEU:H | 2.24 | 0.41 |
| 1:B:233:HIS:HB2 | 1:B:312:ARG:NH1 | 2.35 | 0.41 |
| 1:D:149:MET:O | 1:D:152:TYR:CG | 2.74 | 0.41 |
| 1:C:149:MET:C | 1:C:152:TYR:CZ | 2.94 | 0.41 |
| 1:B:150:PRO:N | 1:B:152:TYR:CE1 | 2.89 | 0.41 |
| 1:C:54:TYR:CD1 | 1:C:118:PRO:HB2 | 2.55 | 0.41 |
| 1:C:91:PHE:CE2 | 1:C:267:GLU:HG3 | 2.56 | 0.41 |
| 1:E:81:ARG:HD2 | 1:E:208:HIS:NE2 | 2.34 | 0.41 |
| 1:C:81:ARG:HD2 | 1:C:208:HIS:NE2 | 2.34 | 0.41 |
| 1:D:303:LEU:CD2 | 1:D:328:THR:HA | 2.51 | 0.41 |
| 1:E:397:ALA:HB1 | 1:E:420:PHE:CG | 2.56 | 0.41 |
| 1:C:18:LEU:HD12 | 1:D:232:GLY:HA2 | 2.02 | 0.41 |
| 1:D:149:MET:C | 1:D:152:TYR:CZ | 2.94 | 0.41 |
| 1:C:153:ARG:CZ | 1:C:176:PRO:HA | 2.51 | 0.41 |
| 1:A:151:GLU:CD | 2:R:33:C:H4' | 2.40 | 0.41 |
| 1:C:134:LEU:HD22 | 1:C:134:LEU:HA | 1.95 | 0.41 |
| 1:A:354:LYS:CE | 1:A:356:THR:HA | 2.40 | 0.41 |
| 1:D:112:ALA:HB1 | 1:D:113:LEU:HD23 | 2.02 | 0.41 |
| 1:C:73:LEU:O | 1:C:74:TYR:C | 2.59 | 0.41 |
| 1:D:78:LYS:HE2 | 1:D:78:LYS:HB2 | 1.74 | 0.41 |
| 1:D:28:PRO:O | 1:D:31:TYR:HB3 | 2.21 | 0.41 |
| 1:E:208:HIS:CE1 | 1:E:210:CYS:HB2 | 2.56 | 0.41 |
| 1:C:86:LYS:HB3 | 1:C:87:ASP:H | 1.59 | 0.41 |
| 1:C:208:HIS:CE1 | 1:C:209:GLU:HG3 | 2.56 | 0.41 |
| 1:A:255:ALA:O | 1:A:259:VAL:HG23 | 2.20 | 0.41 |
| 1:E:295:PRO:HB2 | 1:E:322:ILE:HG21 | 2.03 | 0.41 |
| 1:C:240:MET:HE3 | 1:C:244:ASP:HB3 | 2.03 | 0.41 |
| 1:C:202:PHE:CG | 1:C:211:ALA:HA | 2.56 | 0.41 |
| 1:C:366:THR:C | 1:C:368:ALA:H | 2.23 | 0.41 |
| 1:D:134:LEU:HA | 1:D:134:LEU:HD22 | 1.96 | 0.41 |
| 1:C:123:ASP:C | 1:C:125:SER:H | 2.25 | 0.41 |
| 1:B:215:TYR:C | 1:B:215:TYR:CD2 | 2.94 | 0.41 |
| 1:A:81:ARG:HD2 | 1:A:208:HIS:NE2 | 2.35 | 0.41 |
| 1:A:361:THR:HB | 1:A:362:GLY:H | 1.77 | 0.41 |
| 1:C:150:PRO:N | 1:C:152:TYR:CZ | 2.89 | 0.40 |
| 1:E:53:GLY:O | 1:E:54:TYR:C | 2.59 | 0.40 |
| 1:E:38:ILE:O | 1:E:108:VAL:HB | 2.20 | 0.40 |
| 1:D:31:TYR:CD1 | 1:D:32:PHE:N | 2.88 | 0.40 |
| 1:B:14:ILE:CD1 | 1:C:259:VAL:HA | 2.51 | 0.40 |
| 1:A:303:LEU:CD2 | 1:A:328:THR:HA | 2.51 | 0.40 |
| 1:A:55:VAL:O | 1:A:56:TYR:C | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:240:MET:HE3 | 1:E:244:ASP:CB | 2.51 | 0.40 |
| 1:A:155:LYS:NZ | 2:R:35:C:OP2 | 2.43 | 0.40 |
| 1:C:387:ARG:HB3 | 1:C:387:ARG:CZ | 2.51 | 0.40 |
| 1:C:382:PHE:CD2 | 1:C:387:ARG:HA | 2.56 | 0.40 |
| 1:C:58:GLY:O | 1:C:63:ASN:O | 2.39 | 0.40 |
| 1:B:89:SER:O | 1:B:90:SER:CB | 2.65 | 0.40 |
| 1:A:397:ALA:HB1 | 1:A:420:PHE:CG | 2.57 | 0.40 |
| 1:C:415:TYR:C | 1:C:415:TYR:CD1 | 2.95 | 0.40 |
| 1:E:182:PHE:N | 1:E:182:PHE:CD2 | 2.90 | 0.40 |
| 1:C:151:GLU:HG2 | 1:C:155:LYS:HD3 | 2.03 | 0.40 |
| 1:A:38:ILE:O | 1:A:108:VAL:HB | 2.20 | 0.40 |
| 1:B:31:TYR:CD1 | 1:B:32:PHE:N | 2.89 | 0.40 |
| 1:C:389:PRO:HB3 | 1:C:393:MET:HE3 | 2.03 | 0.40 |
| 1:D:382:PHE:HE1 | 1:D:393:MET:HE2 | 1.86 | 0.40 |
| 1:B:14:ILE:HD12 | 1:C:259:VAL:HG22 | 2.03 | 0.40 |
| 1:D:66:ILE:HD13 | 1:D:185:TRP:CD1 | 2.56 | 0.40 |
| 1:A:308:LEU:HA | 1:A:308:LEU:HD12 | 1.86 | 0.40 |
| 1:B:249:ILE:HD13 | 1:B:254:VAL:HG12 | 2.02 | 0.40 |
| 1:E:202:PHE:CG | 1:E:211:ALA:HA | 2.56 | 0.40 |
| 1:E:153:ARG:HH12 | 1:E:177:GLU:HB2 | 1.87 | 0.40 |
| 1:A:86:LYS:HB3 | 1:A:87:ASP:H | 1.58 | 0.40 |
| 1:E:66:ILE:HD13 | 1:E:185:TRP:CD1 | 2.57 | 0.40 |
| 1:C:93:ILE:HD12 | 1:C:93:ILE:N | 2.37 | 0.40 |
| 1:A:369:PRO:HB3 | 1:A:381:TRP:CZ2 | 2.56 | 0.40 |
| 1:E:215:TYR:CD1 | 2:R:45:C:H5" | 2.56 | 0.40 |
| 1:A:240:MET:HE3 | 1:A:244:ASP:CB | 2.51 | 0.40 |
| 1:A:202:PHE:CG | 1:A:211:ALA:HA | 2.56 | 0.40 |
| 1:C:88:TRP:CZ3 | 1:C:204:MET:HG2 | 2.57 | 0.40 |
| 1:A:421:ASP:O | 1:A:422:LYS:HB3 | 2.20 | 0.40 |
| 1:B:151:GLU:HG2 | 1:B:155:LYS:HD3 | 2.03 | 0.40 |
| 1:E:410:LYS:NZ | 2:R:40:C:N4 | 2.68 | 0.40 |
| 1:E:263:LEU:HD12 | 1:E:263:LEU:HA | 1.91 | 0.40 |
| 1:A:354:LYS:NZ | 1:E:380:GLY:HA2 | 2.37 | 0.40 |
| 1:C:74:TYR:O | 1:C:78:LYS:HD3 | 2.20 | 0.40 |
| 1:A:38:ILE:CD1 | 1:A:107:LEU:O | 2.70 | 0.40 |
| 1:C:37:GLU:CB | 1:C:108:VAL:HG11 | 2.43 | 0.40 |
| 1:B:253:GLU:N | 1:B:253:GLU:CD | 2.71 | 0.40 |
| 1:E:79:ASP:O | 1:E:79:ASP:CG | 2.60 | 0.40 |
| 1:D:309:ARG:HD3 | 1:D:309:ARG:HH11 | 1.78 | 0.40 |
| 1:A:397:ALA:O | 1:A:401:VAL:HG22 | 2.21 | 0.40 |
| 1:B:119:ASP:OD1 | 1:B:119:ASP:N | 2.55 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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 | |
|-----|-------|-----------------|------------|-----------|----------|-------------|---|
| 1 | A | 419/421 (100%) | 306 (73%) | 82 (20%) | 31 (7%) | 1 | 7 |
| 1 | B | 411/421 (98%) | 302 (74%) | 73 (18%) | 36 (9%) | 1 | 5 |
| 1 | C | 409/421 (97%) | 296 (72%) | 73 (18%) | 40 (10%) | 1 | 4 |
| 1 | D | 412/421 (98%) | 303 (74%) | 75 (18%) | 34 (8%) | 1 | 6 |
| 1 | E | 419/421 (100%) | 303 (72%) | 76 (18%) | 40 (10%) | 1 | 4 |
| All | All | 2070/2105 (98%) | 1510 (73%) | 379 (18%) | 181 (9%) | 1 | 5 |

All (181) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 43 | ASN |
| 1 | A | 44 | THR |
| 1 | A | 60 | LYS |
| 1 | A | 61 | SER |
| 1 | A | 79 | ASP |
| 1 | A | 90 | SER |
| 1 | A | 131 | ASP |
| 1 | A | 150 | PRO |
| 1 | B | 43 | ASN |
| 1 | B | 60 | LYS |
| 1 | B | 61 | SER |
| 1 | B | 79 | ASP |
| 1 | B | 90 | SER |
| 1 | B | 131 | ASP |
| 1 | B | 150 | PRO |
| 1 | B | 168 | ASN |
| 1 | B | 169 | GLU |
| 1 | C | 43 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 60 | LYS |
| 1 | C | 79 | ASP |
| 1 | C | 90 | SER |
| 1 | C | 131 | ASP |
| 1 | C | 150 | PRO |
| 1 | C | 170 | GLN |
| 1 | D | 43 | ASN |
| 1 | D | 44 | THR |
| 1 | D | 60 | LYS |
| 1 | D | 61 | SER |
| 1 | D | 79 | ASP |
| 1 | D | 90 | SER |
| 1 | D | 131 | ASP |
| 1 | D | 271 | ALA |
| 1 | E | 43 | ASN |
| 1 | E | 60 | LYS |
| 1 | E | 61 | SER |
| 1 | E | 79 | ASP |
| 1 | E | 90 | SER |
| 1 | E | 131 | ASP |
| 1 | E | 150 | PRO |
| 1 | E | 271 | ALA |
| 1 | E | 360 | SER |
| 1 | E | 365 | THR |
| 1 | A | 4 | THR |
| 1 | A | 30 | ASP |
| 1 | A | 84 | LEU |
| 1 | A | 100 | ASP |
| 1 | A | 172 | GLU |
| 1 | A | 173 | PRO |
| 1 | A | 271 | ALA |
| 1 | B | 4 | THR |
| 1 | B | 30 | ASP |
| 1 | B | 44 | THR |
| 1 | B | 84 | LEU |
| 1 | B | 100 | ASP |
| 1 | B | 170 | GLN |
| 1 | B | 173 | PRO |
| 1 | B | 176 | PRO |
| 1 | B | 208 | HIS |
| 1 | B | 271 | ALA |
| 1 | B | 344 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 4 | THR |
| 1 | C | 30 | ASP |
| 1 | C | 44 | THR |
| 1 | C | 61 | SER |
| 1 | C | 100 | ASP |
| 1 | C | 172 | GLU |
| 1 | C | 173 | PRO |
| 1 | C | 176 | PRO |
| 1 | C | 208 | HIS |
| 1 | C | 271 | ALA |
| 1 | C | 343 | ASP |
| 1 | D | 4 | THR |
| 1 | D | 30 | ASP |
| 1 | D | 84 | LEU |
| 1 | D | 100 | ASP |
| 1 | D | 150 | PRO |
| 1 | D | 171 | PHE |
| 1 | D | 172 | GLU |
| 1 | D | 173 | PRO |
| 1 | D | 176 | PRO |
| 1 | D | 208 | HIS |
| 1 | E | 4 | THR |
| 1 | E | 44 | THR |
| 1 | E | 84 | LEU |
| 1 | E | 100 | ASP |
| 1 | E | 164 | CYS |
| 1 | E | 168 | ASN |
| 1 | E | 172 | GLU |
| 1 | E | 173 | PRO |
| 1 | E | 208 | HIS |
| 1 | A | 28 | PRO |
| 1 | A | 81 | ARG |
| 1 | A | 112 | ALA |
| 1 | A | 117 | LEU |
| 1 | A | 129 | ALA |
| 1 | A | 176 | PRO |
| 1 | A | 177 | GLU |
| 1 | A | 208 | HIS |
| 1 | A | 343 | ASP |
| 1 | A | 344 | LEU |
| 1 | B | 63 | ASN |
| 1 | B | 81 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 112 | ALA |
| 1 | B | 117 | LEU |
| 1 | B | 172 | GLU |
| 1 | B | 177 | GLU |
| 1 | C | 28 | PRO |
| 1 | C | 81 | ARG |
| 1 | C | 84 | LEU |
| 1 | C | 112 | ALA |
| 1 | C | 117 | LEU |
| 1 | C | 168 | ASN |
| 1 | C | 177 | GLU |
| 1 | C | 345 | ALA |
| 1 | D | 81 | ARG |
| 1 | D | 112 | ALA |
| 1 | D | 117 | LEU |
| 1 | D | 177 | GLU |
| 1 | D | 344 | LEU |
| 1 | E | 28 | PRO |
| 1 | E | 30 | ASP |
| 1 | E | 81 | ARG |
| 1 | E | 88 | TRP |
| 1 | E | 112 | ALA |
| 1 | E | 117 | LEU |
| 1 | E | 129 | ALA |
| 1 | E | 171 | PHE |
| 1 | E | 176 | PRO |
| 1 | E | 177 | GLU |
| 1 | E | 343 | ASP |
| 1 | E | 344 | LEU |
| 1 | B | 343 | ASP |
| 1 | C | 108 | VAL |
| 1 | C | 167 | ILE |
| 1 | C | 344 | LEU |
| 1 | D | 28 | PRO |
| 1 | D | 108 | VAL |
| 1 | D | 206 | LYS |
| 1 | D | 343 | ASP |
| 1 | A | 23 | ASP |
| 1 | A | 88 | TRP |
| 1 | A | 108 | VAL |
| 1 | A | 123 | ASP |
| 1 | B | 23 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 28 | PRO |
| 1 | B | 88 | TRP |
| 1 | B | 108 | VAL |
| 1 | B | 123 | ASP |
| 1 | C | 23 | ASP |
| 1 | C | 88 | TRP |
| 1 | C | 129 | ALA |
| 1 | C | 206 | LYS |
| 1 | C | 228 | LEU |
| 1 | D | 23 | ASP |
| 1 | D | 63 | ASN |
| 1 | D | 88 | TRP |
| 1 | D | 123 | ASP |
| 1 | D | 167 | ILE |
| 1 | E | 23 | ASP |
| 1 | E | 108 | VAL |
| 1 | E | 123 | ASP |
| 1 | E | 363 | GLY |
| 1 | E | 364 | LEU |
| 1 | A | 206 | LYS |
| 1 | B | 239 | GLY |
| 1 | C | 63 | ASN |
| 1 | C | 123 | ASP |
| 1 | C | 174 | LEU |
| 1 | D | 106 | ASP |
| 1 | E | 174 | LEU |
| 1 | C | 239 | GLY |
| 1 | B | 219 | VAL |
| 1 | B | 16 | PRO |
| 1 | C | 16 | PRO |
| 1 | C | 219 | VAL |
| 1 | D | 219 | VAL |
| 1 | A | 16 | PRO |
| 1 | B | 19 | PRO |
| 1 | E | 167 | ILE |
| 1 | E | 219 | VAL |
| 1 | E | 16 | PRO |

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 | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1 | A | 362/362 (100%) | 298 (82%) | 64 (18%) | 2 | 10 |
| 1 | B | 358/362 (99%) | 293 (82%) | 65 (18%) | 2 | 9 |
| 1 | C | 356/362 (98%) | 294 (83%) | 62 (17%) | 2 | 11 |
| 1 | D | 359/362 (99%) | 296 (82%) | 63 (18%) | 2 | 10 |
| 1 | E | 362/362 (100%) | 300 (83%) | 62 (17%) | 2 | 11 |
| All | All | 1797/1810 (99%) | 1481 (82%) | 316 (18%) | 2 | 10 |

All (316) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 3 | VAL |
| 1 | A | 8 | ILE |
| 1 | A | 13 | VAL |
| 1 | A | 18 | LEU |
| 1 | A | 25 | VAL |
| 1 | A | 31 | TYR |
| 1 | A | 36 | LYS |
| 1 | A | 40 | LEU |
| 1 | A | 69 | VAL |
| 1 | A | 70 | ASN |
| 1 | A | 84 | LEU |
| 1 | A | 97 | LYS |
| 1 | A | 100 | ASP |
| 1 | A | 101 | THR |
| 1 | A | 117 | LEU |
| 1 | A | 119 | ASP |
| 1 | A | 123 | ASP |
| 1 | A | 126 | ARG |
| 1 | A | 134 | LEU |
| 1 | A | 148 | GLN |
| 1 | A | 152 | TYR |
| 1 | A | 153 | ARG |
| 1 | A | 156 | LEU |
| 1 | A | 160 | LEU |
| 1 | A | 162 | ASN |
| 1 | A | 169 | GLU |
| 1 | A | 170 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 172 | GLU |
| 1 | A | 174 | LEU |
| 1 | A | 175 | VAL |
| 1 | A | 180 | ASP |
| 1 | A | 181 | ILE |
| 1 | A | 183 | ASP |
| 1 | A | 187 | ASN |
| 1 | A | 209 | GLU |
| 1 | A | 217 | THR |
| 1 | A | 228 | LEU |
| 1 | A | 230 | THR |
| 1 | A | 241 | SER |
| 1 | A | 242 | THR |
| 1 | A | 243 | GLU |
| 1 | A | 252 | ARG |
| 1 | A | 253 | GLU |
| 1 | A | 268 | ILE |
| 1 | A | 291 | SER |
| 1 | A | 307 | LEU |
| 1 | A | 308 | LEU |
| 1 | A | 311 | THR |
| 1 | A | 317 | ARG |
| 1 | A | 325 | THR |
| 1 | A | 327 | LEU |
| 1 | A | 332 | LEU |
| 1 | A | 352 | ASP |
| 1 | A | 356 | THR |
| 1 | A | 358 | ASP |
| 1 | A | 359 | ASP |
| 1 | A | 361 | THR |
| 1 | A | 364 | LEU |
| 1 | A | 365 | THR |
| 1 | A | 384 | ASP |
| 1 | A | 385 | GLN |
| 1 | A | 405 | GLN |
| 1 | A | 410 | LYS |
| 1 | A | 414 | LYS |
| 1 | B | 3 | VAL |
| 1 | B | 8 | ILE |
| 1 | B | 13 | VAL |
| 1 | B | 18 | LEU |
| 1 | B | 25 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 31 | TYR |
| 1 | B | 36 | LYS |
| 1 | B | 40 | LEU |
| 1 | B | 57 | GLN |
| 1 | B | 69 | VAL |
| 1 | B | 70 | ASN |
| 1 | B | 84 | LEU |
| 1 | B | 97 | LYS |
| 1 | B | 100 | ASP |
| 1 | B | 101 | THR |
| 1 | B | 107 | LEU |
| 1 | B | 117 | LEU |
| 1 | B | 119 | ASP |
| 1 | B | 123 | ASP |
| 1 | B | 126 | ARG |
| 1 | B | 134 | LEU |
| 1 | B | 148 | GLN |
| 1 | B | 152 | TYR |
| 1 | B | 153 | ARG |
| 1 | B | 156 | LEU |
| 1 | B | 160 | LEU |
| 1 | B | 162 | ASN |
| 1 | B | 169 | GLU |
| 1 | B | 170 | GLN |
| 1 | B | 172 | GLU |
| 1 | B | 174 | LEU |
| 1 | B | 175 | VAL |
| 1 | B | 180 | ASP |
| 1 | B | 181 | ILE |
| 1 | B | 183 | ASP |
| 1 | B | 187 | ASN |
| 1 | B | 209 | GLU |
| 1 | B | 217 | THR |
| 1 | B | 228 | LEU |
| 1 | B | 230 | THR |
| 1 | B | 241 | SER |
| 1 | B | 242 | THR |
| 1 | B | 243 | GLU |
| 1 | B | 252 | ARG |
| 1 | B | 253 | GLU |
| 1 | B | 268 | ILE |
| 1 | B | 291 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 307 | LEU |
| 1 | B | 308 | LEU |
| 1 | B | 311 | THR |
| 1 | B | 317 | ARG |
| 1 | B | 325 | THR |
| 1 | B | 327 | LEU |
| 1 | B | 332 | LEU |
| 1 | B | 352 | ASP |
| 1 | B | 354 | LYS |
| 1 | B | 356 | THR |
| 1 | B | 358 | ASP |
| 1 | B | 365 | THR |
| 1 | B | 366 | THR |
| 1 | B | 384 | ASP |
| 1 | B | 385 | GLN |
| 1 | B | 405 | GLN |
| 1 | B | 410 | LYS |
| 1 | B | 414 | LYS |
| 1 | C | 3 | VAL |
| 1 | C | 8 | ILE |
| 1 | C | 13 | VAL |
| 1 | C | 18 | LEU |
| 1 | C | 25 | VAL |
| 1 | C | 31 | TYR |
| 1 | C | 36 | LYS |
| 1 | C | 40 | LEU |
| 1 | C | 57 | GLN |
| 1 | C | 69 | VAL |
| 1 | C | 70 | ASN |
| 1 | C | 84 | LEU |
| 1 | C | 97 | LYS |
| 1 | C | 100 | ASP |
| 1 | C | 101 | THR |
| 1 | C | 107 | LEU |
| 1 | C | 117 | LEU |
| 1 | C | 119 | ASP |
| 1 | C | 123 | ASP |
| 1 | C | 126 | ARG |
| 1 | C | 134 | LEU |
| 1 | C | 148 | GLN |
| 1 | C | 152 | TYR |
| 1 | C | 153 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 156 | LEU |
| 1 | C | 160 | LEU |
| 1 | C | 162 | ASN |
| 1 | C | 167 | ILE |
| 1 | C | 169 | GLU |
| 1 | C | 170 | GLN |
| 1 | C | 172 | GLU |
| 1 | C | 174 | LEU |
| 1 | C | 175 | VAL |
| 1 | C | 180 | ASP |
| 1 | C | 181 | ILE |
| 1 | C | 183 | ASP |
| 1 | C | 187 | ASN |
| 1 | C | 209 | GLU |
| 1 | C | 217 | THR |
| 1 | C | 228 | LEU |
| 1 | C | 230 | THR |
| 1 | C | 241 | SER |
| 1 | C | 242 | THR |
| 1 | C | 243 | GLU |
| 1 | C | 252 | ARG |
| 1 | C | 253 | GLU |
| 1 | C | 268 | ILE |
| 1 | C | 291 | SER |
| 1 | C | 308 | LEU |
| 1 | C | 311 | THR |
| 1 | C | 317 | ARG |
| 1 | C | 325 | THR |
| 1 | C | 327 | LEU |
| 1 | C | 332 | LEU |
| 1 | C | 352 | ASP |
| 1 | C | 353 | ASN |
| 1 | C | 356 | THR |
| 1 | C | 384 | ASP |
| 1 | C | 385 | GLN |
| 1 | C | 405 | GLN |
| 1 | C | 410 | LYS |
| 1 | C | 414 | LYS |
| 1 | D | 3 | VAL |
| 1 | D | 8 | ILE |
| 1 | D | 13 | VAL |
| 1 | D | 18 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 25 | VAL |
| 1 | D | 31 | TYR |
| 1 | D | 36 | LYS |
| 1 | D | 40 | LEU |
| 1 | D | 57 | GLN |
| 1 | D | 69 | VAL |
| 1 | D | 70 | ASN |
| 1 | D | 84 | LEU |
| 1 | D | 97 | LYS |
| 1 | D | 100 | ASP |
| 1 | D | 101 | THR |
| 1 | D | 117 | LEU |
| 1 | D | 119 | ASP |
| 1 | D | 123 | ASP |
| 1 | D | 126 | ARG |
| 1 | D | 134 | LEU |
| 1 | D | 148 | GLN |
| 1 | D | 152 | TYR |
| 1 | D | 153 | ARG |
| 1 | D | 156 | LEU |
| 1 | D | 160 | LEU |
| 1 | D | 162 | ASN |
| 1 | D | 167 | ILE |
| 1 | D | 169 | GLU |
| 1 | D | 172 | GLU |
| 1 | D | 174 | LEU |
| 1 | D | 175 | VAL |
| 1 | D | 180 | ASP |
| 1 | D | 181 | ILE |
| 1 | D | 183 | ASP |
| 1 | D | 187 | ASN |
| 1 | D | 209 | GLU |
| 1 | D | 217 | THR |
| 1 | D | 228 | LEU |
| 1 | D | 230 | THR |
| 1 | D | 242 | THR |
| 1 | D | 243 | GLU |
| 1 | D | 252 | ARG |
| 1 | D | 253 | GLU |
| 1 | D | 268 | ILE |
| 1 | D | 291 | SER |
| 1 | D | 307 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 308 | LEU |
| 1 | D | 311 | THR |
| 1 | D | 317 | ARG |
| 1 | D | 325 | THR |
| 1 | D | 327 | LEU |
| 1 | D | 332 | LEU |
| 1 | D | 352 | ASP |
| 1 | D | 353 | ASN |
| 1 | D | 354 | LYS |
| 1 | D | 356 | THR |
| 1 | D | 358 | ASP |
| 1 | D | 366 | THR |
| 1 | D | 384 | ASP |
| 1 | D | 385 | GLN |
| 1 | D | 405 | GLN |
| 1 | D | 410 | LYS |
| 1 | D | 414 | LYS |
| 1 | E | 8 | ILE |
| 1 | E | 13 | VAL |
| 1 | E | 18 | LEU |
| 1 | E | 25 | VAL |
| 1 | E | 31 | TYR |
| 1 | E | 36 | LYS |
| 1 | E | 40 | LEU |
| 1 | E | 57 | GLN |
| 1 | E | 69 | VAL |
| 1 | E | 70 | ASN |
| 1 | E | 84 | LEU |
| 1 | E | 97 | LYS |
| 1 | E | 100 | ASP |
| 1 | E | 101 | THR |
| 1 | E | 117 | LEU |
| 1 | E | 119 | ASP |
| 1 | E | 123 | ASP |
| 1 | E | 126 | ARG |
| 1 | E | 134 | LEU |
| 1 | E | 148 | GLN |
| 1 | E | 152 | TYR |
| 1 | E | 153 | ARG |
| 1 | E | 156 | LEU |
| 1 | E | 160 | LEU |
| 1 | E | 162 | ASN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 172 | GLU |
| 1 | E | 174 | LEU |
| 1 | E | 175 | VAL |
| 1 | E | 180 | ASP |
| 1 | E | 181 | ILE |
| 1 | E | 183 | ASP |
| 1 | E | 187 | ASN |
| 1 | E | 209 | GLU |
| 1 | E | 217 | THR |
| 1 | E | 228 | LEU |
| 1 | E | 230 | THR |
| 1 | E | 242 | THR |
| 1 | E | 243 | GLU |
| 1 | E | 252 | ARG |
| 1 | E | 253 | GLU |
| 1 | E | 268 | ILE |
| 1 | E | 272 | ASP |
| 1 | E | 291 | SER |
| 1 | E | 308 | LEU |
| 1 | E | 311 | THR |
| 1 | E | 317 | ARG |
| 1 | E | 325 | THR |
| 1 | E | 327 | LEU |
| 1 | E | 332 | LEU |
| 1 | E | 352 | ASP |
| 1 | E | 353 | ASN |
| 1 | E | 354 | LYS |
| 1 | E | 356 | THR |
| 1 | E | 358 | ASP |
| 1 | E | 359 | ASP |
| 1 | E | 365 | THR |
| 1 | E | 366 | THR |
| 1 | E | 384 | ASP |
| 1 | E | 385 | GLN |
| 1 | E | 405 | GLN |
| 1 | E | 410 | LYS |
| 1 | E | 414 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 11 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 57 | GLN |
| 1 | A | 70 | ASN |
| 1 | A | 170 | GLN |
| 1 | A | 203 | HIS |
| 1 | A | 260 | GLN |
| 1 | A | 266 | GLN |
| 1 | A | 347 | GLN |
| 1 | A | 386 | ASN |
| 1 | B | 11 | ASN |
| 1 | B | 57 | GLN |
| 1 | B | 70 | ASN |
| 1 | B | 168 | ASN |
| 1 | B | 170 | GLN |
| 1 | B | 190 | ASN |
| 1 | B | 203 | HIS |
| 1 | B | 260 | GLN |
| 1 | B | 266 | GLN |
| 1 | B | 347 | GLN |
| 1 | B | 386 | ASN |
| 1 | C | 11 | ASN |
| 1 | C | 57 | GLN |
| 1 | C | 70 | ASN |
| 1 | C | 170 | GLN |
| 1 | C | 203 | HIS |
| 1 | C | 260 | GLN |
| 1 | C | 266 | GLN |
| 1 | C | 347 | GLN |
| 1 | C | 386 | ASN |
| 1 | D | 11 | ASN |
| 1 | D | 57 | GLN |
| 1 | D | 70 | ASN |
| 1 | D | 168 | ASN |
| 1 | D | 203 | HIS |
| 1 | D | 266 | GLN |
| 1 | D | 347 | GLN |
| 1 | D | 386 | ASN |
| 1 | E | 11 | ASN |
| 1 | E | 57 | GLN |
| 1 | E | 70 | ASN |
| 1 | E | 203 | HIS |
| 1 | E | 260 | GLN |
| 1 | E | 266 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 347 | GLN |

5.3.3 RNA ⓘ

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 2 | R | 44/45 (97%) | 18 (40%) | 2 (4%) |

All (18) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | R | 3 | C |
| 2 | R | 5 | C |
| 2 | R | 10 | C |
| 2 | R | 13 | C |
| 2 | R | 17 | C |
| 2 | R | 18 | C |
| 2 | R | 19 | C |
| 2 | R | 22 | C |
| 2 | R | 23 | C |
| 2 | R | 25 | C |
| 2 | R | 28 | C |
| 2 | R | 30 | C |
| 2 | R | 31 | C |
| 2 | R | 40 | C |
| 2 | R | 41 | C |
| 2 | R | 42 | C |
| 2 | R | 44 | C |
| 2 | R | 45 | C |

All (2) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | R | 18 | C |
| 2 | R | 41 | C |

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 20 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 | A | 421/421 (100%) | 0.31 | 34 (8%) 15 5 | 70, 102, 138, 158 | 0 |
| 1 | B | 415/421 (98%) | 0.15 | 14 (3%) 49 24 | 71, 101, 137, 157 | 0 |
| 1 | C | 413/421 (98%) | 0.26 | 23 (5%) 28 11 | 71, 101, 137, 158 | 0 |
| 1 | D | 416/421 (98%) | 0.27 | 24 (5%) 26 11 | 71, 102, 137, 158 | 0 |
| 1 | E | 421/421 (100%) | 0.38 | 39 (9%) 11 4 | 70, 102, 140, 163 | 0 |
| 2 | R | 45/45 (100%) | -0.01 | 0 100 100 | 97, 110, 120, 121 | 0 |
| All | All | 2131/2150 (99%) | 0.27 | 134 (6%) 23 9 | 70, 102, 138, 163 | 0 |

All (134) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 2 | SER | 17.4 |
| 1 | E | 2 | SER | 15.2 |
| 1 | C | 2 | SER | 10.2 |
| 1 | B | 2 | SER | 10.2 |
| 1 | A | 362 | GLY | 8.6 |
| 1 | D | 2 | SER | 7.8 |
| 1 | A | 361 | THR | 7.7 |
| 1 | A | 353 | ASN | 6.6 |
| 1 | A | 83 | LYS | 5.9 |
| 1 | E | 363 | GLY | 5.9 |
| 1 | E | 112 | ALA | 5.7 |
| 1 | E | 362 | GLY | 5.7 |
| 1 | C | 83 | LYS | 5.2 |
| 1 | D | 158 | ASP | 5.0 |
| 1 | D | 113 | LEU | 4.9 |
| 1 | E | 95 | ILE | 4.7 |
| 1 | A | 363 | GLY | 4.7 |
| 1 | C | 121 | VAL | 4.6 |
| 1 | E | 101 | THR | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | C | 96 | GLY | 4.3 |
| 1 | C | 101 | THR | 4.3 |
| 1 | D | 166 | MET | 4.2 |
| 1 | C | 353 | ASN | 4.2 |
| 1 | A | 102 | ILE | 4.1 |
| 1 | A | 82 | GLY | 4.1 |
| 1 | C | 98 | ALA | 4.1 |
| 1 | A | 98 | ALA | 4.0 |
| 1 | E | 365 | THR | 4.0 |
| 1 | A | 122 | SER | 3.8 |
| 1 | E | 98 | ALA | 3.8 |
| 1 | E | 62 | GLY | 3.7 |
| 1 | E | 113 | LEU | 3.7 |
| 1 | E | 121 | VAL | 3.7 |
| 1 | D | 274 | TYR | 3.6 |
| 1 | B | 62 | GLY | 3.6 |
| 1 | E | 96 | GLY | 3.5 |
| 1 | D | 371 | GLN | 3.5 |
| 1 | C | 99 | GLY | 3.5 |
| 1 | E | 88 | TRP | 3.4 |
| 1 | A | 121 | VAL | 3.4 |
| 1 | A | 355 | TYR | 3.4 |
| 1 | B | 274 | TYR | 3.3 |
| 1 | A | 95 | ILE | 3.2 |
| 1 | E | 43 | ASN | 3.2 |
| 1 | A | 85 | ASP | 3.2 |
| 1 | D | 346 | GLN | 3.2 |
| 1 | E | 158 | ASP | 3.2 |
| 1 | A | 365 | THR | 3.2 |
| 1 | A | 360 | SER | 3.2 |
| 1 | A | 357 | PRO | 3.1 |
| 1 | A | 96 | GLY | 3.1 |
| 1 | E | 44 | THR | 3.0 |
| 1 | E | 97 | LYS | 3.0 |
| 1 | A | 269 | ASP | 3.0 |
| 1 | E | 361 | THR | 3.0 |
| 1 | D | 43 | ASN | 3.0 |
| 1 | A | 84 | LEU | 3.0 |
| 1 | C | 97 | LYS | 3.0 |
| 1 | D | 215 | TYR | 3.0 |
| 1 | D | 68 | HIS | 3.0 |
| 1 | B | 42 | ILE | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 359 | ASP | 2.9 |
| 1 | D | 97 | LYS | 2.9 |
| 1 | A | 367 | ASN | 2.9 |
| 1 | E | 355 | TYR | 2.9 |
| 1 | E | 274 | TYR | 2.9 |
| 1 | C | 367 | ASN | 2.9 |
| 1 | E | 57 | GLN | 2.8 |
| 1 | B | 118 | PRO | 2.8 |
| 1 | B | 158 | ASP | 2.8 |
| 1 | D | 33 | ARG | 2.8 |
| 1 | C | 216 | GLY | 2.8 |
| 1 | D | 147 | THR | 2.8 |
| 1 | A | 99 | GLY | 2.7 |
| 1 | E | 42 | ILE | 2.7 |
| 1 | E | 118 | PRO | 2.7 |
| 1 | A | 148 | GLN | 2.7 |
| 1 | C | 84 | LEU | 2.6 |
| 1 | C | 215 | TYR | 2.6 |
| 1 | B | 112 | ALA | 2.6 |
| 1 | C | 82 | GLY | 2.6 |
| 1 | D | 112 | ALA | 2.6 |
| 1 | C | 95 | ILE | 2.6 |
| 1 | A | 62 | GLY | 2.6 |
| 1 | E | 216 | GLY | 2.6 |
| 1 | B | 113 | LEU | 2.6 |
| 1 | D | 353 | ASN | 2.5 |
| 1 | D | 355 | TYR | 2.5 |
| 1 | A | 101 | THR | 2.5 |
| 1 | E | 99 | GLY | 2.5 |
| 1 | A | 158 | ASP | 2.5 |
| 1 | E | 114 | ASP | 2.5 |
| 1 | B | 68 | HIS | 2.5 |
| 1 | C | 168 | ASN | 2.5 |
| 1 | E | 56 | TYR | 2.5 |
| 1 | E | 3 | VAL | 2.4 |
| 1 | D | 13 | VAL | 2.4 |
| 1 | E | 83 | LYS | 2.4 |
| 1 | C | 355 | TYR | 2.4 |
| 1 | A | 364 | LEU | 2.4 |
| 1 | B | 172 | GLU | 2.3 |
| 1 | D | 122 | SER | 2.3 |
| 1 | A | 215 | TYR | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 215 | TYR | 2.3 |
| 1 | A | 356 | THR | 2.3 |
| 1 | D | 367 | ASN | 2.3 |
| 1 | E | 33 | ARG | 2.3 |
| 1 | C | 14 | ILE | 2.2 |
| 1 | A | 45 | THR | 2.2 |
| 1 | D | 27 | TYR | 2.2 |
| 1 | C | 148 | GLN | 2.2 |
| 1 | E | 63 | ASN | 2.2 |
| 1 | E | 207 | LYS | 2.2 |
| 1 | D | 114 | ASP | 2.2 |
| 1 | E | 117 | LEU | 2.2 |
| 1 | D | 102 | ILE | 2.2 |
| 1 | E | 109 | SER | 2.2 |
| 1 | C | 346 | GLN | 2.2 |
| 1 | B | 88 | TRP | 2.2 |
| 1 | A | 358 | ASP | 2.2 |
| 1 | E | 94 | ASN | 2.2 |
| 1 | C | 357 | PRO | 2.1 |
| 1 | C | 88 | TRP | 2.1 |
| 1 | B | 147 | THR | 2.1 |
| 1 | E | 172 | GLU | 2.1 |
| 1 | E | 215 | TYR | 2.1 |
| 1 | B | 365 | THR | 2.1 |
| 1 | E | 364 | LEU | 2.1 |
| 1 | D | 278 | LEU | 2.0 |
| 1 | D | 149 | MET | 2.0 |
| 1 | A | 3 | VAL | 2.0 |
| 1 | E | 166 | MET | 2.0 |
| 1 | A | 206 | LYS | 2.0 |
| 1 | C | 213 | PHE | 2.0 |

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 3 | IUM | E | 534 | 1/3 | 0.99 | 0.17 | -0.14 | 132,132,132,132 | 0 |
| 3 | IUM | A | 522 | 1/3 | 1.00 | 0.14 | -0.51 | 129,129,129,129 | 0 |
| 3 | IUM | C | 529 | 1/3 | 0.98 | 0.13 | -0.83 | 136,136,136,136 | 0 |
| 3 | IUM | B | 526 | 1/3 | 1.00 | 0.16 | -1.80 | 125,125,125,125 | 0 |
| 3 | IUM | D | 532 | 1/3 | 1.00 | 0.15 | -2.38 | 125,125,125,125 | 0 |
| 3 | IUM | D | 531 | 1/3 | 0.94 | 0.10 | - | 156,156,156,156 | 1 |
| 3 | IUM | D | 530 | 1/3 | 0.92 | 0.08 | - | 166,166,166,166 | 1 |
| 3 | IUM | B | 527 | 1/3 | 0.81 | 0.10 | - | 156,156,156,156 | 1 |
| 3 | IUM | R | 536 | 1/3 | 0.99 | 0.14 | - | 130,130,130,130 | 0 |
| 3 | IUM | R | 537 | 1/3 | 0.99 | 0.15 | - | 122,122,122,122 | 1 |
| 3 | IUM | B | 525 | 1/3 | 0.97 | 0.09 | - | 134,134,134,134 | 1 |
| 3 | IUM | E | 533 | 1/3 | 0.97 | 0.11 | - | 132,132,132,132 | 1 |
| 3 | IUM | A | 523 | 1/3 | 0.95 | 0.12 | - | 175,175,175,175 | 1 |
| 3 | IUM | A | 521 | 1/3 | 0.95 | 0.10 | - | 132,132,132,132 | 1 |
| 3 | IUM | R | 538 | 1/3 | 0.99 | 0.13 | - | 126,126,126,126 | 0 |
| 3 | IUM | B | 524 | 1/3 | 0.92 | 0.09 | - | 165,165,165,165 | 1 |
| 3 | IUM | R | 540 | 1/3 | 1.00 | 0.16 | - | 126,126,126,126 | 1 |
| 3 | IUM | C | 528 | 1/3 | 0.98 | 0.10 | - | 136,136,136,136 | 1 |
| 3 | IUM | R | 539 | 1/3 | 0.98 | 0.14 | - | 112,112,112,112 | 1 |
| 3 | IUM | E | 535 | 1/3 | 0.87 | 0.07 | - | 160,160,160,160 | 1 |

6.5 Other polymers [i](#)

There are no such residues in this entry.