



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:15 PM GMT

PDB ID : 4KXF
Title : Crystal structure of NLRC4 reveals its autoinhibition mechanism
Authors : Chai, J.; Hu, Z.
Deposited on : 2013-05-25
Resolution : 3.20 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

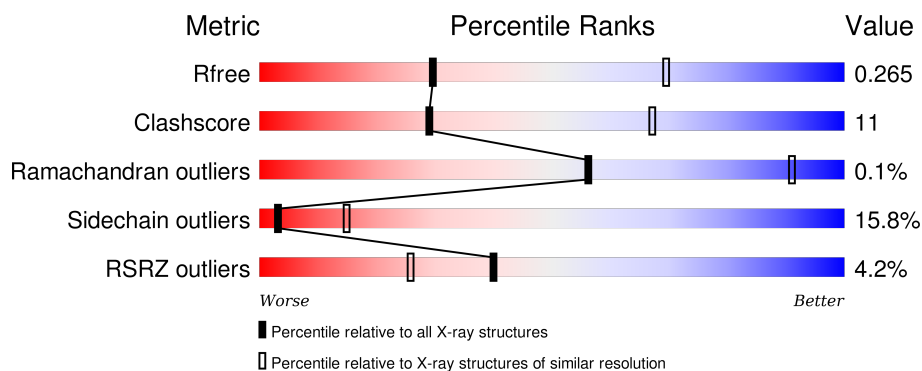
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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 | 1124 (3.24-3.16) |
| Clashscore | 102246 | 1024 (3.22-3.18) |
| Ramachandran outliers | 100387 | 1004 (3.22-3.18) |
| Sidechain outliers | 100360 | 1003 (3.22-3.18) |
| RSRZ outliers | 91569 | 1129 (3.24-3.16) |

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 | B | 1024 | <div> <div>2%</div> <div>57%</div> <div>26%</div> <div>5%</div> <div>12%</div> </div> |
| 1 | D | 1024 | <div> <div>3%</div> <div>59%</div> <div>26%</div> <div>•</div> <div>12%</div> </div> |
| 1 | F | 1024 | <div> <div>3%</div> <div>58%</div> <div>25%</div> <div>•</div> <div>12%</div> </div> |
| 1 | H | 1024 | <div> <div>3%</div> <div>57%</div> <div>27%</div> <div>•</div> <div>12%</div> </div> |
| 1 | K | 1024 | <div> <div>2%</div> <div>56%</div> <div>28%</div> <div>•</div> <div>12%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | L | 1024 | |
| 1 | N | 1024 | |
| 1 | P | 1024 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3 | SO4 | B | 1102 | - | - | - | X |

2 Entry composition

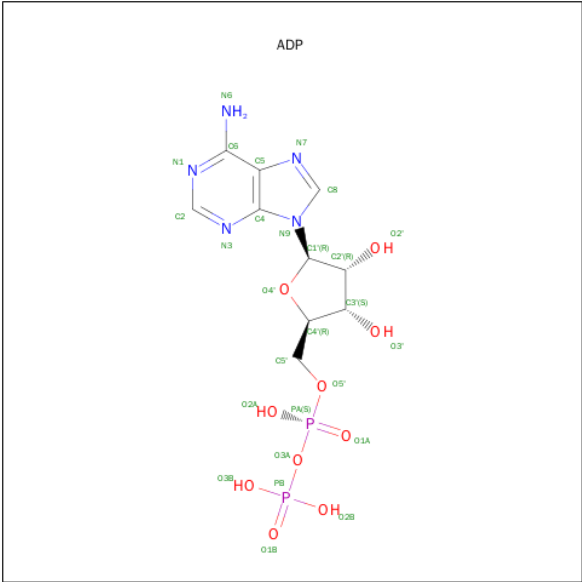
There are 3 unique types of molecules in this entry. The entry contains 57081 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NLR family CARD domain-containing protein 4.

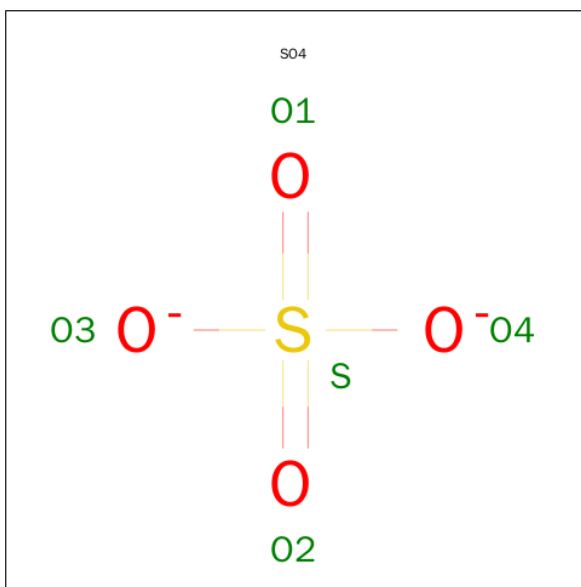
| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|----|---------|---------|-------|
| 1 | K | 904 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 7208 | 4600 | 1215 | 1352 | 1 | 40 | | | |
| 1 | B | 903 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 7204 | 4599 | 1222 | 1342 | 1 | 40 | | | |
| 1 | D | 900 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 7177 | 4581 | 1208 | 1347 | 1 | 40 | | | |
| 1 | F | 899 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 7172 | 4577 | 1208 | 1346 | 1 | 40 | | | |
| 1 | H | 898 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 7135 | 4553 | 1201 | 1340 | 1 | 40 | | | |
| 1 | L | 893 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 7107 | 4540 | 1199 | 1327 | 1 | 40 | | | |
| 1 | N | 882 | Total | C | N | O | S | | 0 | 0 | 0 |
| | | | 6996 | 4468 | 1181 | 1307 | 40 | | | | |
| 1 | P | 866 | Total | C | N | O | S | | 0 | 0 | 0 |
| | | | 6856 | 4377 | 1157 | 1282 | 40 | | | | |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2 | K | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | F | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | H | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | L | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | N | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | P | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

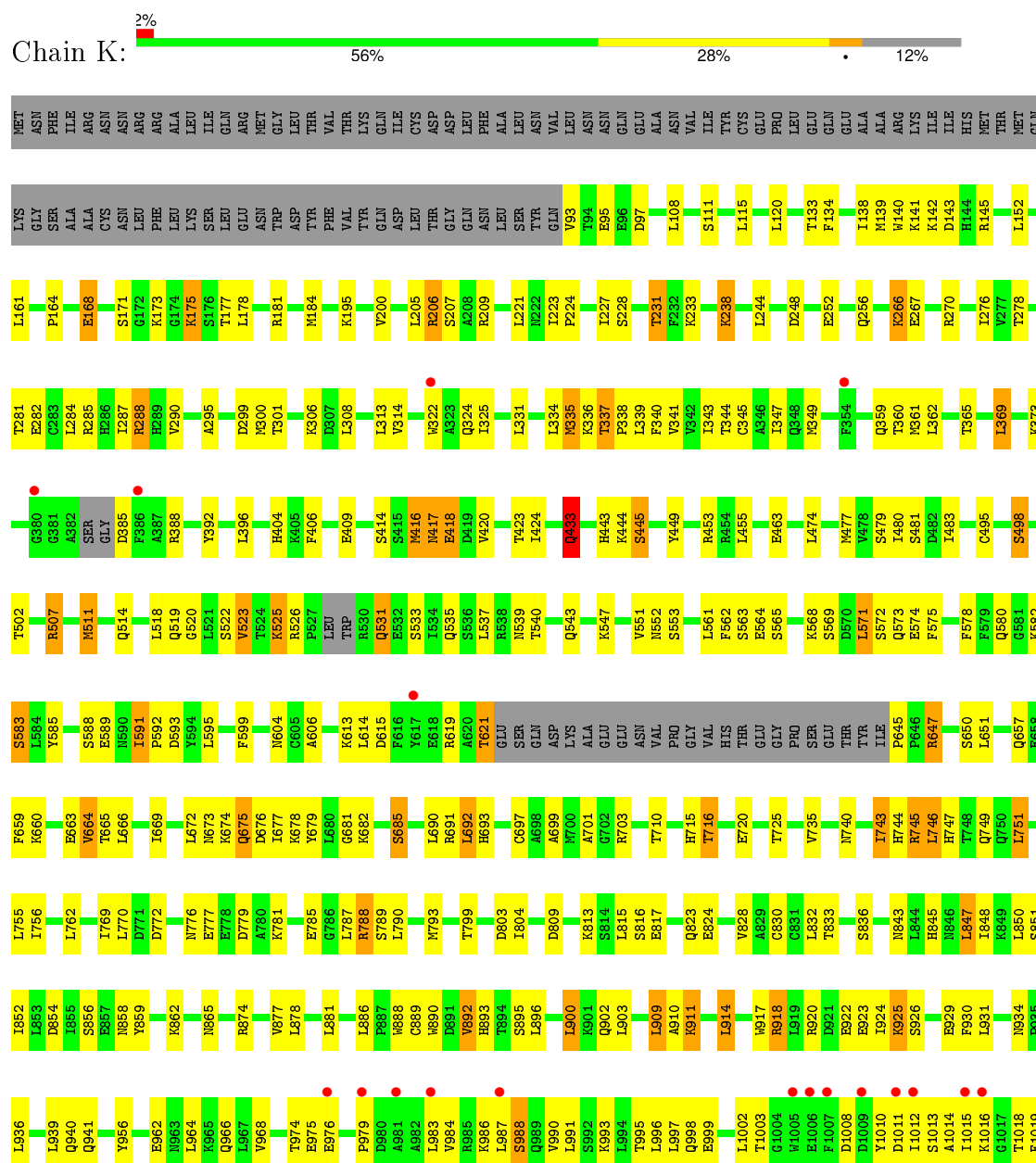


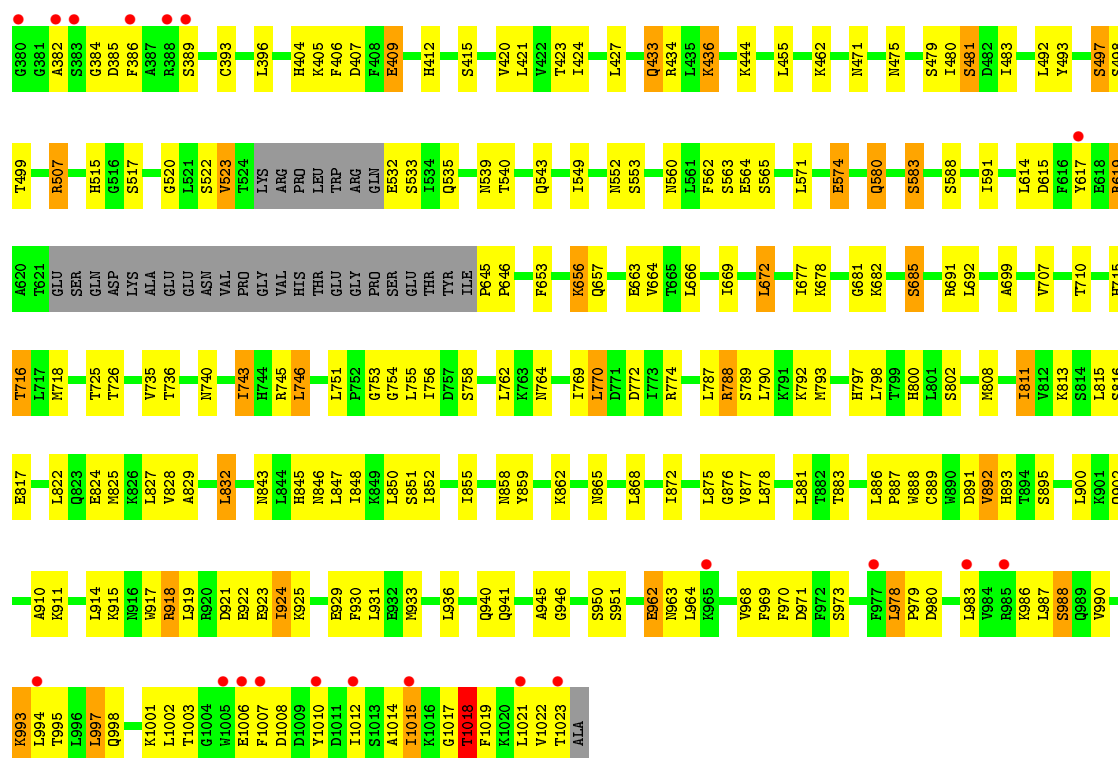
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | N | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

3 Residue-property plots

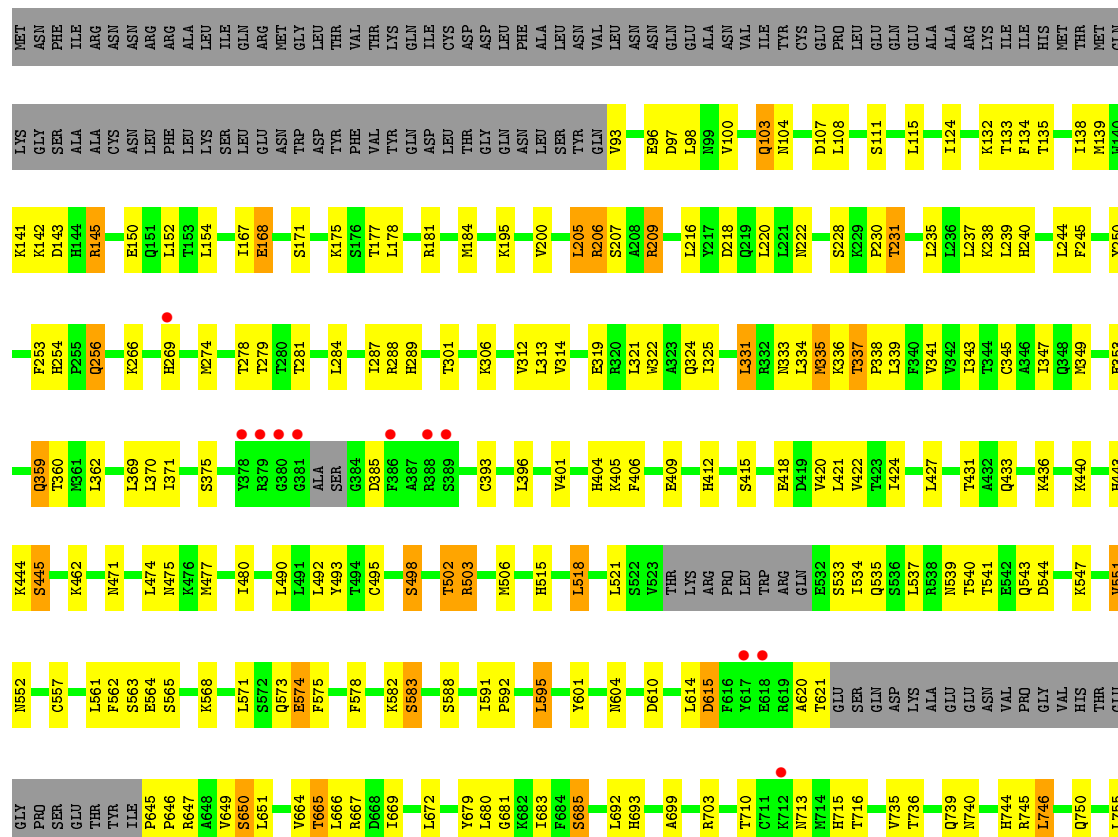
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

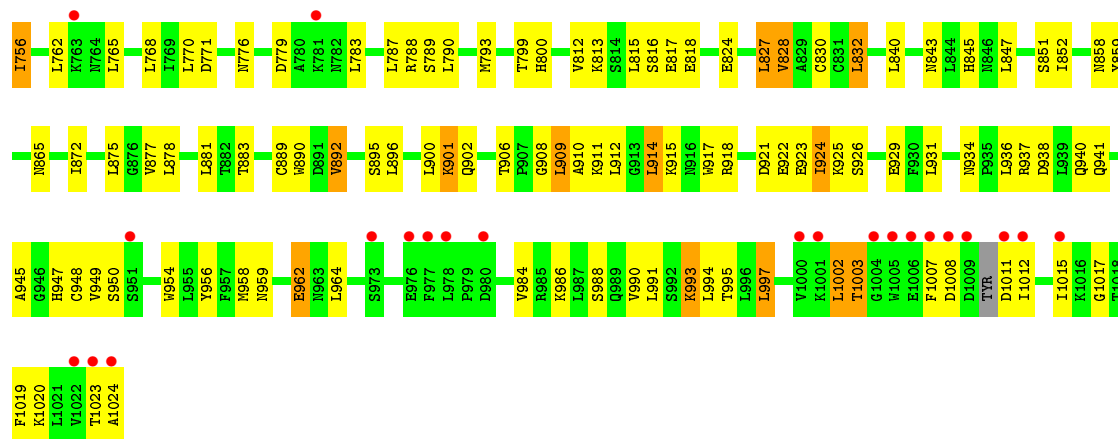
- Molecule 1: NLR family CARD domain-containing protein 4



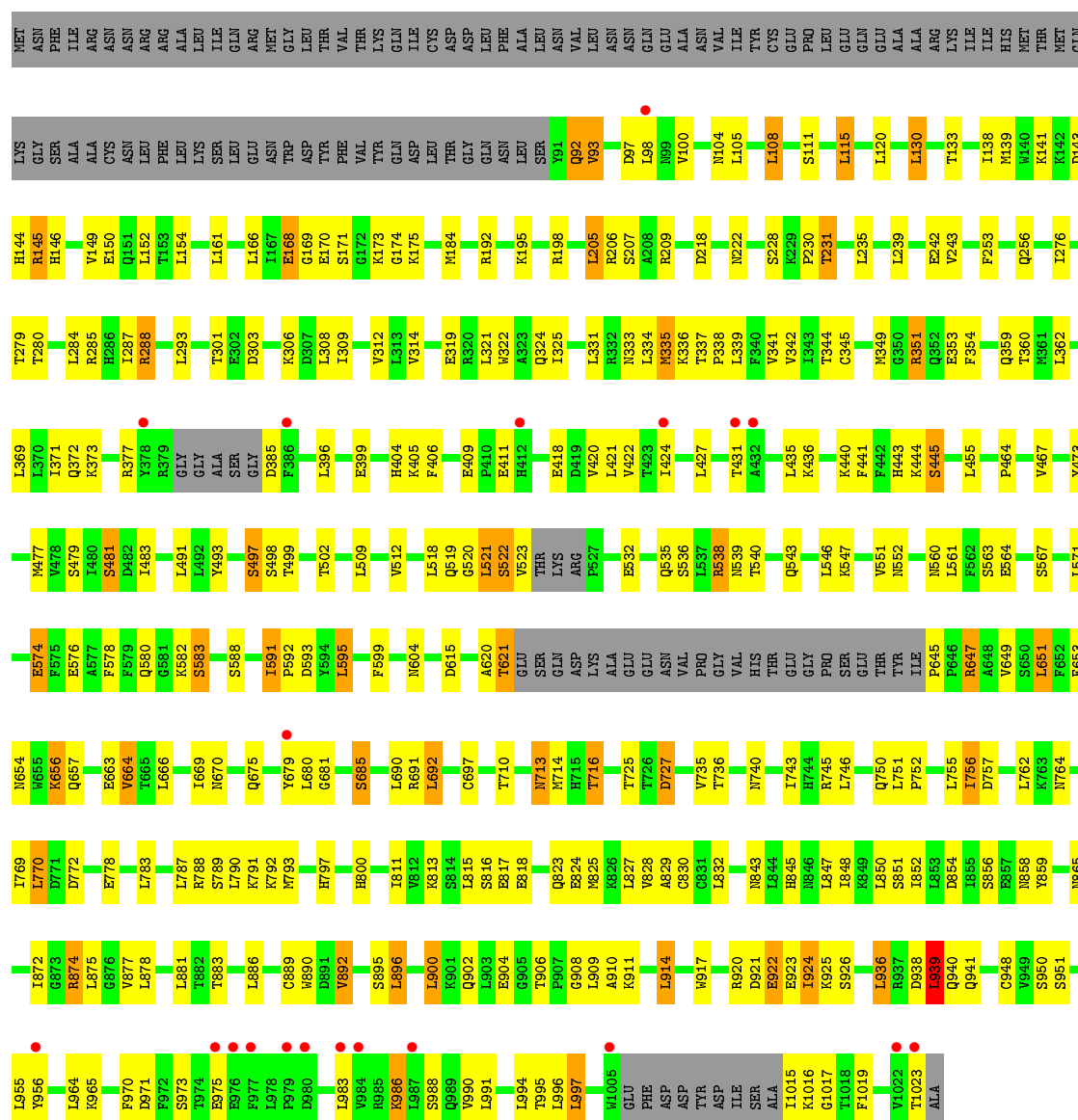


• Molecule 1: NLR family CARD domain-containing protein 4

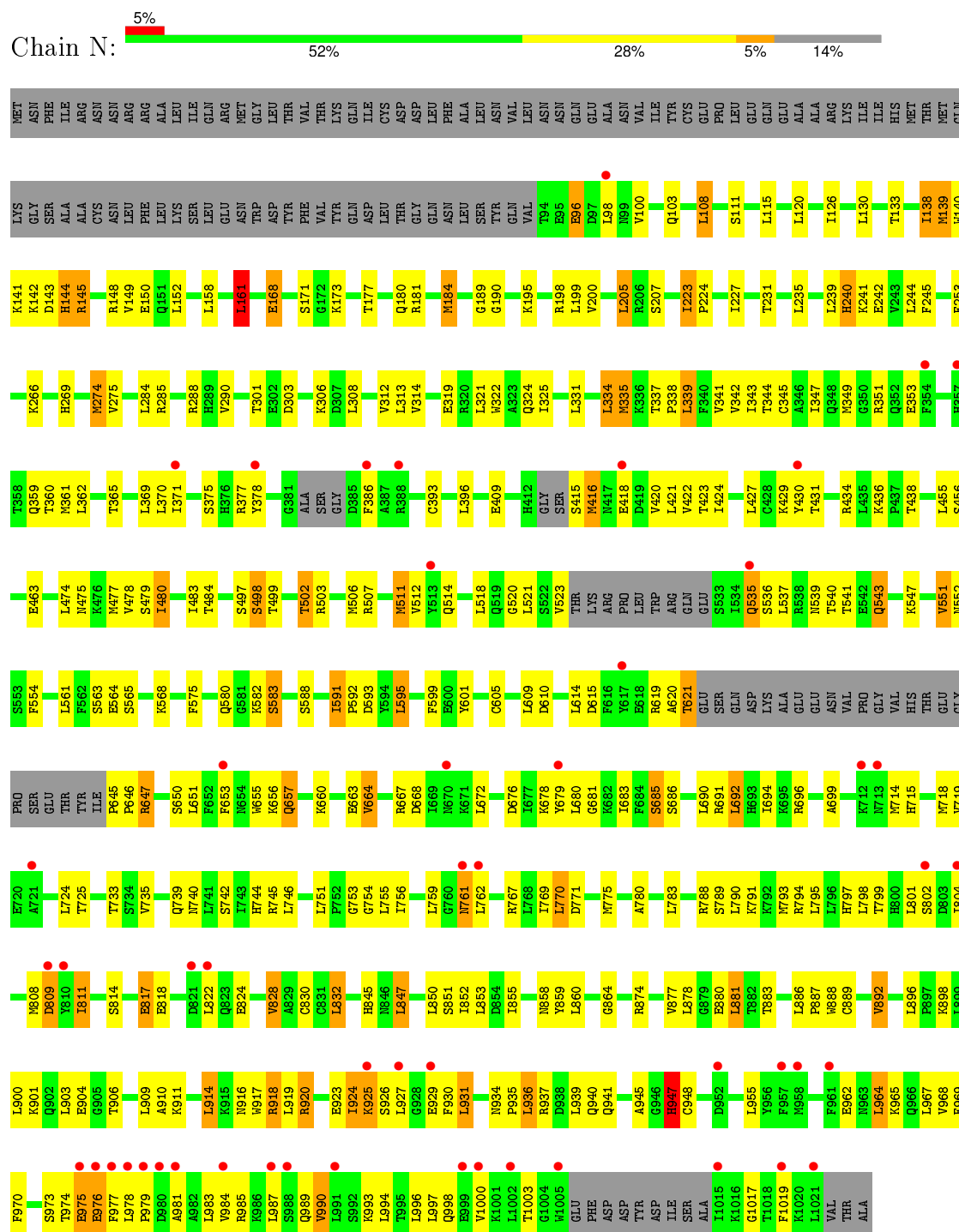




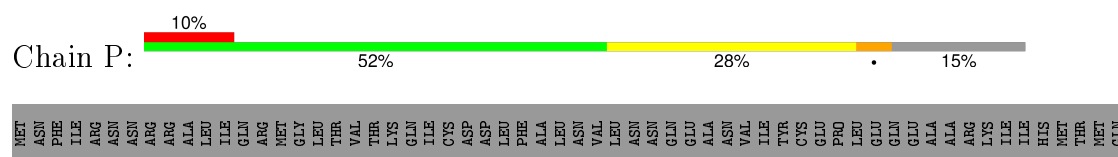
• Molecule 1: NLR family CARD domain-containing protein 4

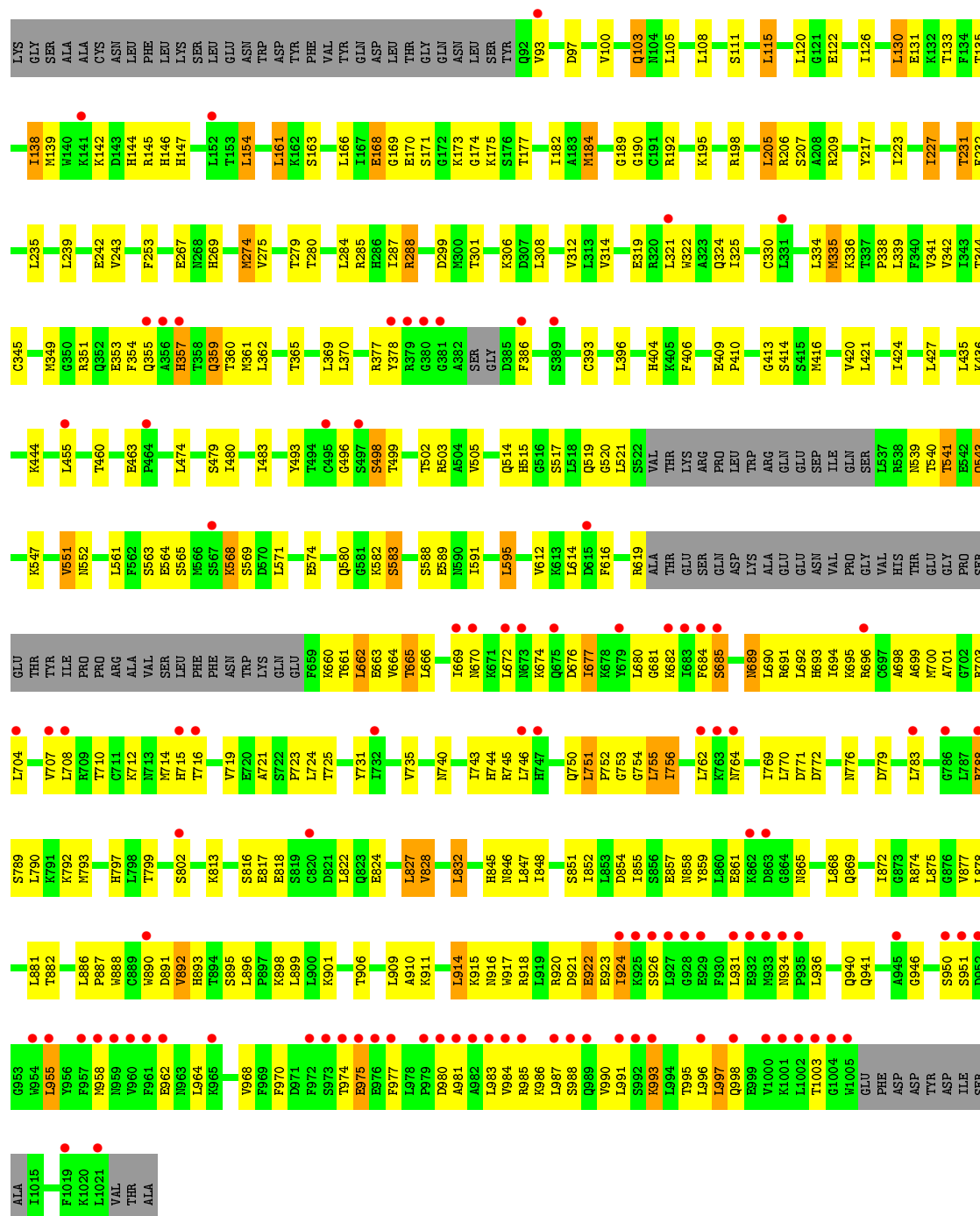


• Molecule 1: NLR family CARD domain-containing protein 4



• Molecule 1: NLR family CARD domain-containing protein 4





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 41 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 334.05Å 334.05Å 177.57Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 39.33 – 3.20 39.33 – 3.18 | Depositor EDS |
| % Data completeness (in resolution range) | 90.9 (39.33-3.20) 89.8 (39.33-3.18) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.11 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.84 (at 3.18Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.8_1069) | Depositor |
| R, R_{free} | 0.226 , 0.266 0.226 , 0.265 | Depositor DCC |
| R_{free} test set | 7523 reflections (5.04%) | DCC |
| Wilson B-factor (Å ²) | 78.8 | Xtriage |
| Anisotropy | 0.007 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 19.3 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Outliers | 2 of 150157 reflections (0.001%) | Xtriage |
| F_o, F_c correlation | 0.91 | EDS |
| Total number of atoms | 57081 | wwPDB-VP |
| Average B, all atoms (Å ²) | 31.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.31% 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: SO4, ADP, SEP

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 | B | 0.28 | 0/7330 | 0.58 | 1/9897 (0.0%) |
| 1 | D | 0.27 | 0/7301 | 0.53 | 0/9857 |
| 1 | F | 0.26 | 0/7296 | 0.52 | 0/9851 |
| 1 | H | 0.26 | 0/7256 | 0.53 | 0/9798 |
| 1 | K | 0.27 | 0/7332 | 0.57 | 2/9900 (0.0%) |
| 1 | L | 0.28 | 0/7230 | 0.54 | 2/9766 (0.0%) |
| 1 | N | 0.30 | 0/7119 | 0.59 | 2/9616 (0.0%) |
| 1 | P | 0.27 | 0/6980 | 0.55 | 1/9426 (0.0%) |
| All | All | 0.27 | 0/57844 | 0.55 | 8/78111 (0.0%) |

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 | B | 0 | 1 |
| 1 | F | 0 | 1 |
| 1 | K | 0 | 1 |
| 1 | L | 0 | 1 |
| All | All | 0 | 4 |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | K | 433 | GLN | OE1-CD-NE2 | -15.42 | 86.42 | 121.90 |
| 1 | N | 978 | LEU | N-CA-C | -7.16 | 91.66 | 111.00 |
| 1 | N | 161 | LEU | CA-CB-CG | 6.39 | 130.01 | 115.30 |
| 1 | B | 161 | LEU | CA-CB-CG | 6.26 | 129.69 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1 | P | 161 | LEU | CA-CB-CG | 5.76 | 128.56 | 115.30 |
| 1 | K | 751 | LEU | CA-CB-CG | 5.18 | 127.22 | 115.30 |
| 1 | L | 874 | ARG | NE-CZ-NH1 | 5.11 | 122.86 | 120.30 |
| 1 | L | 939 | LEU | CA-CB-CG | 5.02 | 126.84 | 115.30 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | B | 531 | GLN | Peptide |
| 1 | F | 412 | HIS | Peptide |
| 1 | K | 433 | GLN | Sidechain |
| 1 | L | 92 | GLN | 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 | B | 7204 | 0 | 7237 | 163 | 0 |
| 1 | D | 7177 | 0 | 7190 | 148 | 0 |
| 1 | F | 7172 | 0 | 7186 | 168 | 0 |
| 1 | H | 7135 | 0 | 7126 | 156 | 0 |
| 1 | K | 7208 | 0 | 7216 | 172 | 2 |
| 1 | L | 7107 | 0 | 7104 | 158 | 0 |
| 1 | N | 6996 | 0 | 6969 | 197 | 0 |
| 1 | P | 6856 | 0 | 6838 | 166 | 0 |
| 2 | B | 27 | 0 | 12 | 1 | 0 |
| 2 | D | 27 | 0 | 12 | 1 | 0 |
| 2 | F | 27 | 0 | 12 | 1 | 0 |
| 2 | H | 27 | 0 | 12 | 0 | 0 |
| 2 | K | 27 | 0 | 12 | 2 | 0 |
| 2 | L | 27 | 0 | 12 | 1 | 0 |
| 2 | N | 27 | 0 | 12 | 0 | 0 |
| 2 | P | 27 | 0 | 12 | 2 | 0 |
| 3 | B | 5 | 0 | 0 | 0 | 0 |
| 3 | N | 5 | 0 | 0 | 0 | 0 |
| All | All | 57081 | 0 | 56962 | 1297 | 2 |

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 11.

All (1297) 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:P:983:LEU:HA | 1:P:986:LYS:CB | 1.44 | 1.46 |
| 1:P:983:LEU:O | 1:P:987:LEU:N | 1.59 | 1.32 |
| 1:N:947:HIS:CE1 | 1:N:974:THR:OG1 | 1.92 | 1.22 |
| 1:P:983:LEU:CA | 1:P:986:LYS:CB | 2.32 | 1.06 |
| 1:L:145:ARG:HG2 | 1:L:523:VAL:HG11 | 1.39 | 1.01 |
| 1:L:145:ARG:HG2 | 1:L:523:VAL:CG1 | 1.89 | 1.00 |
| 1:P:981:ALA:HA | 1:P:984:VAL:HB | 1.55 | 0.86 |
| 1:N:916:ASN:H | 1:N:945:ALA:HB3 | 1.39 | 0.85 |
| 1:N:947:HIS:ND1 | 1:N:974:THR:OG1 | 2.08 | 0.85 |
| 1:N:285:ARG:HH21 | 1:N:521:LEU:HD21 | 1.42 | 0.84 |
| 1:N:981:ALA:O | 1:N:985:ARG:N | 2.10 | 0.84 |
| 1:K:984:VAL:HG11 | 1:K:1011:ASP:HB3 | 1.60 | 0.82 |
| 1:N:975:GLU:OE2 | 1:N:975:GLU:HA | 1.67 | 0.82 |
| 1:N:620:ALA:HB1 | 1:N:680:LEU:HD11 | 1.62 | 0.82 |
| 1:K:716:THR:HB | 1:K:740:ASN:HB2 | 1.61 | 0.81 |
| 1:P:93:VAL:HG22 | 1:P:231:THR:HG22 | 1.62 | 0.81 |
| 1:H:845:HIS:HA | 1:H:877:VAL:HG11 | 1.63 | 0.80 |
| 1:D:142:LYS:NZ | 1:D:296:GLU:OE1 | 2.15 | 0.80 |
| 1:F:788:ARG:NH2 | 1:F:817:GLU:OE1 | 2.15 | 0.79 |
| 1:D:205:LEU:HD21 | 1:D:247:LEU:HB3 | 1.65 | 0.79 |
| 1:P:955:LEU:HD12 | 1:P:983:LEU:CB | 2.13 | 0.78 |
| 1:B:591:ILE:O | 1:B:647:ARG:NH1 | 2.15 | 0.78 |
| 1:P:962:GLU:HG3 | 1:P:990:VAL:HG13 | 1.66 | 0.78 |
| 1:K:911:LYS:HG3 | 1:K:941:GLN:HG2 | 1.66 | 0.78 |
| 1:N:975:GLU:OE2 | 1:N:975:GLU:CA | 2.29 | 0.78 |
| 1:H:908:GLY:HA2 | 1:H:938:ASP:HB2 | 1.67 | 0.77 |
| 1:H:788:ARG:NH2 | 1:H:817:GLU:OE1 | 2.18 | 0.77 |
| 1:P:983:LEU:O | 1:P:986:LYS:CA | 2.33 | 0.76 |
| 1:L:145:ARG:CG | 1:L:523:VAL:HG11 | 2.14 | 0.76 |
| 1:N:808:MET:HA | 1:N:811:ILE:HG23 | 1.67 | 0.76 |
| 1:B:522:SER:HB3 | 1:B:525:LYS:HG3 | 1.65 | 0.75 |
| 1:L:921:ASP:OD1 | 1:L:950:SER:OG | 2.04 | 0.75 |
| 1:K:344:THR:HG22 | 1:K:362:LEU:HD11 | 1.66 | 0.75 |
| 1:K:591:ILE:O | 1:K:647:ARG:NH1 | 2.19 | 0.75 |
| 1:P:745:ARG:HA | 1:P:772:ASP:HB3 | 1.69 | 0.75 |
| 1:N:830:CYS:O | 1:N:858:ASN:ND2 | 2.18 | 0.75 |
| 1:H:962:GLU:HG2 | 1:H:993:LYS:HE3 | 1.68 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:L:874:ARG:HG3 | 1:L:874:ARG:HH11 | 1.52 | 0.73 |
| 1:N:783:LEU:HD21 | 1:N:798:LEU:HD22 | 1.70 | 0.73 |
| 1:N:975:GLU:O | 1:N:976:GLU:CB | 2.29 | 0.73 |
| 1:D:205:LEU:HB3 | 1:D:253:PHE:HB2 | 1.68 | 0.73 |
| 1:P:719:VAL:HB | 1:P:743:ILE:HG22 | 1.71 | 0.73 |
| 1:F:285:ARG:NH1 | 1:F:517:SER:O | 2.22 | 0.73 |
| 1:P:788:ARG:NH1 | 1:P:817:GLU:OE2 | 2.22 | 0.73 |
| 1:N:756:ILE:HD11 | 1:N:783:LEU:HB2 | 1.71 | 0.73 |
| 1:D:620:ALA:HB1 | 1:D:680:LEU:HD11 | 1.71 | 0.73 |
| 1:K:531:GLN:HG2 | 1:K:769:ILE:HD13 | 1.70 | 0.73 |
| 1:H:672:LEU:HB2 | 1:H:699:ALA:HB1 | 1.71 | 0.73 |
| 1:L:591:ILE:O | 1:L:647:ARG:NH1 | 2.21 | 0.72 |
| 1:P:921:ASP:OD1 | 1:P:950:SER:OG | 2.07 | 0.72 |
| 1:L:716:THR:HB | 1:L:740:ASN:HB2 | 1.71 | 0.72 |
| 1:P:816:SER:O | 1:P:846:ASN:ND2 | 2.22 | 0.72 |
| 1:P:845:HIS:HA | 1:P:877:VAL:HG11 | 1.69 | 0.72 |
| 1:B:288:ARG:NH2 | 1:B:522:SER:O | 2.23 | 0.72 |
| 1:F:816:SER:O | 1:F:846:ASN:ND2 | 2.22 | 0.72 |
| 1:D:830:CYS:O | 1:D:858:ASN:ND2 | 2.23 | 0.72 |
| 1:B:816:SER:HB2 | 1:B:843:ASN:HB2 | 1.71 | 0.72 |
| 1:K:621:THR:OG1 | 1:K:676:ASP:OD1 | 2.08 | 0.72 |
| 1:H:620:ALA:HB1 | 1:H:680:LEU:HD11 | 1.71 | 0.72 |
| 1:L:908:GLY:HA2 | 1:L:938:ASP:HB2 | 1.72 | 0.71 |
| 1:B:621:THR:OG1 | 1:B:676:ASP:OD1 | 2.08 | 0.71 |
| 1:K:284:LEU:HG | 1:K:288:ARG:HG3 | 1.72 | 0.71 |
| 1:P:716:THR:HG22 | 1:P:740:ASN:HD22 | 1.54 | 0.71 |
| 1:F:552:ASN:OD1 | 1:F:583:SER:OG | 2.09 | 0.71 |
| 1:L:170:GLU:O | 1:L:175:LYS:NZ | 2.24 | 0.70 |
| 1:B:701:ALA:O | 1:B:725:THR:OG1 | 2.07 | 0.70 |
| 1:N:973:SER:O | 1:N:974:THR:OG1 | 2.09 | 0.70 |
| 1:L:681:GLY:O | 1:L:685:SER:OG | 2.09 | 0.70 |
| 1:B:1002:LEU:HD23 | 1:B:1007:PHE:HE2 | 1.55 | 0.70 |
| 1:B:184:MET:O | 1:B:188:SER:OG | 2.10 | 0.70 |
| 1:H:592:PRO:HD2 | 1:H:595:LEU:HD23 | 1.74 | 0.70 |
| 1:K:675:GLN:HA | 1:K:678:LYS:HE2 | 1.74 | 0.70 |
| 1:L:552:ASN:OD1 | 1:L:583:SER:OG | 2.11 | 0.69 |
| 1:L:334:LEU:HD23 | 1:L:362:LEU:HD22 | 1.75 | 0.69 |
| 1:P:324:GLN:HE22 | 1:P:354:PHE:H | 1.40 | 0.69 |
| 1:F:344:THR:HG23 | 1:F:362:LEU:HD11 | 1.74 | 0.69 |
| 1:K:526:ARG:HD2 | 1:K:999:GLU:HB2 | 1.75 | 0.69 |
| 1:P:983:LEU:O | 1:P:986:LYS:C | 2.29 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:98:LEU:HD13 | 1:L:235:LEU:HD11 | 1.74 | 0.69 |
| 1:P:170:GLU:O | 1:P:175:LYS:NZ | 2.25 | 0.69 |
| 1:K:369:LEU:HD22 | 1:K:373:LYS:HD3 | 1.75 | 0.69 |
| 1:N:591:ILE:O | 1:N:647:ARG:NH1 | 2.26 | 0.68 |
| 1:P:958:MET:HB3 | 1:P:990:VAL:HG21 | 1.75 | 0.68 |
| 1:N:974:THR:HG22 | 1:N:975:GLU:H | 1.58 | 0.68 |
| 1:D:911:LYS:HG2 | 1:D:941:GLN:HG2 | 1.74 | 0.68 |
| 1:D:463:GLU:HG3 | 1:F:774:ARG:HH22 | 1.58 | 0.68 |
| 1:H:256:GLN:HG2 | 1:L:230:PRO:HG3 | 1.75 | 0.68 |
| 1:P:324:GLN:NE2 | 1:P:354:PHE:O | 2.27 | 0.68 |
| 1:P:93:VAL:HG21 | 1:P:235:LEU:HB2 | 1.76 | 0.68 |
| 1:D:383:SER:OG | 1:D:384:GLY:N | 2.26 | 0.68 |
| 1:F:288:ARG:NH1 | 1:F:522:SER:O | 2.26 | 0.68 |
| 1:P:515:HIS:CD2 | 1:P:547:LYS:HD3 | 2.28 | 0.67 |
| 1:K:845:HIS:HA | 1:K:877:VAL:HG11 | 1.77 | 0.67 |
| 1:F:334:LEU:HD13 | 1:F:362:LEU:HD22 | 1.76 | 0.67 |
| 1:P:163:SER:HB2 | 1:P:274:MET:HE3 | 1.77 | 0.67 |
| 1:K:788:ARG:NH1 | 1:K:817:GLU:OE1 | 2.27 | 0.67 |
| 1:B:256:GLN:HG2 | 1:F:230:PRO:HG3 | 1.77 | 0.67 |
| 1:B:592:PRO:HD2 | 1:B:595:LEU:HD23 | 1.76 | 0.67 |
| 1:K:552:ASN:OD1 | 1:K:583:SER:OG | 2.12 | 0.67 |
| 1:B:681:GLY:O | 1:B:685:SER:OG | 2.13 | 0.66 |
| 1:L:920:ARG:NH2 | 1:L:922:GLU:OE1 | 2.28 | 0.66 |
| 1:K:228:SER:HG | 1:K:231:THR:HG1 | 1.39 | 0.66 |
| 1:N:552:ASN:OD1 | 1:N:583:SER:OG | 2.13 | 0.66 |
| 1:N:920:ARG:HG2 | 1:N:923:GLU:HG2 | 1.77 | 0.66 |
| 1:F:142:LYS:NZ | 1:F:296:GLU:OE1 | 2.29 | 0.66 |
| 1:D:344:THR:HG22 | 1:D:362:LEU:HD11 | 1.78 | 0.66 |
| 1:B:896:LEU:HD12 | 1:B:923:GLU:HB3 | 1.77 | 0.66 |
| 1:P:174:GLY:N | 2:P:1101:ADP:O3B | 2.28 | 0.66 |
| 1:N:224:PRO:HB2 | 1:N:227:ILE:HG13 | 1.78 | 0.66 |
| 1:K:681:GLY:O | 1:K:685:SER:OG | 2.13 | 0.66 |
| 1:K:824:GLU:HG2 | 1:K:852:ILE:HB | 1.77 | 0.66 |
| 1:F:285:ARG:NH1 | 1:F:481:SER:OG | 2.30 | 0.65 |
| 1:N:918:ARG:NH2 | 1:N:948:CYS:SG | 2.61 | 0.65 |
| 1:N:98:LEU:HD11 | 1:N:199:LEU:HD11 | 1.77 | 0.65 |
| 1:P:983:LEU:O | 1:P:986:LYS:N | 2.29 | 0.65 |
| 1:L:166:LEU:HD22 | 1:L:287:ILE:HD12 | 1.78 | 0.65 |
| 1:D:540:THR:HG23 | 1:D:541:THR:HG22 | 1.78 | 0.65 |
| 1:K:417:ASN:N | 1:K:417:ASN:OD1 | 2.29 | 0.65 |
| 1:N:975:GLU:OE2 | 1:N:975:GLU:N | 2.30 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:416:MET:SD | 1:N:416:MET:N | 2.68 | 0.65 |
| 1:P:975:GLU:O | 1:P:977:PHE:N | 2.30 | 0.65 |
| 1:L:830:CYS:O | 1:L:858:ASN:ND2 | 2.26 | 0.65 |
| 1:N:681:GLY:O | 1:N:685:SER:OG | 2.14 | 0.65 |
| 1:D:568:LYS:HD3 | 1:D:601:TYR:CZ | 2.31 | 0.65 |
| 1:K:511:MET:O | 1:K:511:MET:HG2 | 1.97 | 0.65 |
| 1:P:227:ILE:HD11 | 1:P:232:PHE:HD1 | 1.60 | 0.65 |
| 1:L:727:ASP:OD2 | 1:L:727:ASP:N | 2.29 | 0.65 |
| 1:B:334:LEU:HD13 | 1:B:362:LEU:HD22 | 1.78 | 0.65 |
| 1:B:228:SER:OG | 1:B:231:THR:OG1 | 2.10 | 0.65 |
| 1:K:968:VAL:HG13 | 1:K:998:GLN:HB2 | 1.78 | 0.64 |
| 1:F:754:GLY:O | 1:F:758:SER:OG | 2.13 | 0.64 |
| 1:P:981:ALA:O | 1:P:984:VAL:N | 2.30 | 0.64 |
| 1:D:325:ILE:HD11 | 1:D:335:MET:HE2 | 1.80 | 0.64 |
| 1:F:533:SEP:O1P | 1:F:535:GLN:NE2 | 2.30 | 0.64 |
| 1:L:592:PRO:HD2 | 1:L:595:LEU:HD22 | 1.80 | 0.64 |
| 1:K:526:ARG:NH2 | 1:K:1020:LYS:HB3 | 2.13 | 0.64 |
| 1:B:963:ASN:HD21 | 1:F:986:LYS:HE3 | 1.62 | 0.64 |
| 1:F:350:GLY:HA3 | 1:F:369:LEU:HD11 | 1.80 | 0.64 |
| 1:F:808:MET:HA | 1:F:811:ILE:HG23 | 1.78 | 0.64 |
| 1:H:98:LEU:HD13 | 1:H:235:LEU:HD11 | 1.80 | 0.63 |
| 1:N:344:THR:HG22 | 1:N:362:LEU:HD11 | 1.80 | 0.63 |
| 1:K:224:PRO:HB2 | 1:K:227:ILE:HG13 | 1.79 | 0.63 |
| 1:N:845:HIS:HA | 1:N:877:VAL:HG11 | 1.79 | 0.63 |
| 1:N:718:MET:HG2 | 1:N:742:SER:HB3 | 1.80 | 0.63 |
| 1:B:284:LEU:HG | 1:B:288:ARG:HG3 | 1.80 | 0.63 |
| 1:B:588:SER:OG | 1:B:615:ASP:O | 2.15 | 0.63 |
| 1:K:325:ILE:HG12 | 1:K:331:LEU:HD23 | 1.78 | 0.63 |
| 1:D:816:SER:O | 1:D:846:ASN:ND2 | 2.31 | 0.63 |
| 1:B:661:THR:HG23 | 1:B:689:ASN:HB3 | 1.80 | 0.63 |
| 1:D:910:ALA:O | 1:D:940:GLN:N | 2.28 | 0.63 |
| 1:L:713:ASN:OD1 | 1:L:713:ASN:N | 2.31 | 0.63 |
| 1:K:787:LEU:HD13 | 1:K:815:LEU:HD21 | 1.80 | 0.62 |
| 1:N:663:GLU:OE2 | 1:N:691:ARG:NH1 | 2.31 | 0.62 |
| 1:F:588:SER:HB2 | 1:F:645:PRO:HD2 | 1.80 | 0.62 |
| 1:L:620:ALA:HB1 | 1:L:680:LEU:HD11 | 1.81 | 0.62 |
| 1:H:145:ARG:NH2 | 1:H:533:SEP:O1P | 2.33 | 0.62 |
| 1:L:851:SER:HA | 1:L:881:LEU:HA | 1.80 | 0.62 |
| 1:H:552:ASN:OD1 | 1:H:583:SER:OG | 2.16 | 0.62 |
| 1:D:962:GLU:HG2 | 1:D:993:LYS:HD2 | 1.80 | 0.62 |
| 1:F:480:ILE:HG12 | 1:F:515:HIS:HA | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:K:663:GLU:OE2 | 1:K:691:ARG:NH1 | 2.32 | 0.62 |
| 1:P:983:LEU:C | 1:P:986:LYS:H | 2.02 | 0.62 |
| 1:D:284:LEU:HG | 1:D:288:ARG:HG3 | 1.80 | 0.62 |
| 1:F:340:PHE:O | 1:F:344:THR:OG1 | 2.17 | 0.62 |
| 1:B:925:LYS:HA | 1:B:956:TYR:HE2 | 1.64 | 0.62 |
| 1:H:1002:LEU:HD23 | 1:H:1007:PHE:HE2 | 1.63 | 0.62 |
| 1:D:852:ILE:HG12 | 1:D:883:THR:HB | 1.82 | 0.62 |
| 1:F:962:GLU:HG2 | 1:F:993:LYS:HD2 | 1.82 | 0.62 |
| 1:B:289:HIS:CD2 | 1:B:290:VAL:HG23 | 2.35 | 0.62 |
| 1:F:206:ARG:HG2 | 1:F:207:SER:N | 2.13 | 0.62 |
| 1:H:824:GLU:HG2 | 1:H:852:ILE:HB | 1.81 | 0.62 |
| 1:N:983:LEU:O | 1:N:987:LEU:HB2 | 2.00 | 0.62 |
| 1:L:845:HIS:HA | 1:L:877:VAL:HG11 | 1.80 | 0.62 |
| 1:F:681:GLY:O | 1:F:685:SER:OG | 2.17 | 0.62 |
| 1:P:743:ILE:HD11 | 1:P:755:LEU:HD11 | 1.81 | 0.61 |
| 1:D:378:TYR:HD1 | 1:D:386:PHE:HD1 | 1.45 | 0.61 |
| 1:N:847:LEU:HD13 | 1:N:850:LEU:HD13 | 1.82 | 0.61 |
| 1:B:163:SER:HB2 | 1:B:274:MET:HE3 | 1.82 | 0.61 |
| 1:B:123:ASP:OD1 | 1:B:377:ARG:NH2 | 2.31 | 0.61 |
| 1:B:526:ARG:HB3 | 1:B:527:PRO:HD3 | 1.82 | 0.61 |
| 1:D:399:GLU:OE1 | 1:D:473:TYR:OH | 2.16 | 0.61 |
| 1:K:809:ASP:OD1 | 1:K:833:THR:OG1 | 2.18 | 0.61 |
| 1:L:205:LEU:HB3 | 1:L:253:PHE:HB2 | 1.80 | 0.61 |
| 1:K:859:TYR:CE1 | 1:K:889:CYS:HA | 2.36 | 0.61 |
| 1:D:267:GLU:OE1 | 1:D:270:ARG:NH1 | 2.33 | 0.61 |
| 1:H:924:ILE:HG12 | 1:H:949:VAL:HG21 | 1.82 | 0.61 |
| 1:F:672:LEU:HB2 | 1:F:699:ALA:HB1 | 1.81 | 0.60 |
| 1:K:335:MET:HE3 | 1:K:341:VAL:HA | 1.83 | 0.60 |
| 1:F:161:LEU:HD11 | 1:F:276:ILE:HD11 | 1.82 | 0.60 |
| 1:N:621:THR:OG1 | 1:N:676:ASP:OD1 | 2.19 | 0.60 |
| 1:P:981:ALA:O | 1:P:985:ARG:N | 2.29 | 0.60 |
| 1:H:108:LEU:O | 1:H:111:SER:OG | 2.20 | 0.60 |
| 1:L:143:ASP:OD2 | 1:L:144:HIS:N | 2.34 | 0.60 |
| 1:D:868:LEU:HD11 | 1:D:886:LEU:HD13 | 1.83 | 0.60 |
| 1:N:809:ASP:N | 1:N:809:ASP:OD2 | 2.35 | 0.60 |
| 1:P:962:GLU:HG2 | 1:P:993:LYS:HD2 | 1.82 | 0.60 |
| 1:L:145:ARG:HG2 | 1:L:523:VAL:CB | 2.31 | 0.60 |
| 1:H:744:HIS:NE2 | 1:H:771:ASP:OD2 | 2.34 | 0.60 |
| 1:P:217:TYR:HA | 1:P:223:ILE:HD13 | 1.83 | 0.60 |
| 1:F:224:PRO:HB2 | 1:F:227:ILE:HG23 | 1.83 | 0.60 |
| 1:K:200:VAL:HG22 | 1:K:244:LEU:HB3 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:154:LEU:HD21 | 1:P:182:ILE:HG12 | 1.83 | 0.60 |
| 1:N:973:SER:C | 1:N:974:THR:OG1 | 2.39 | 0.60 |
| 1:H:666:LEU:HB3 | 1:H:669:ILE:HD12 | 1.84 | 0.60 |
| 1:K:141:LYS:HB2 | 1:K:152:LEU:HD11 | 1.84 | 0.60 |
| 1:F:745:ARG:HA | 1:F:772:ASP:HB3 | 1.84 | 0.60 |
| 1:L:971:ASP:OD1 | 1:L:973:SER:OG | 2.18 | 0.60 |
| 1:D:921:ASP:OD1 | 1:D:950:SER:OG | 2.20 | 0.60 |
| 1:D:971:ASP:OD1 | 1:D:973:SER:OG | 2.19 | 0.60 |
| 1:P:619:ARG:H | 1:P:669:ILE:HG12 | 1.67 | 0.60 |
| 1:B:749:GLN:OE1 | 1:B:750:GLN:N | 2.34 | 0.60 |
| 1:B:614:LEU:HD11 | 1:B:652:PHE:HZ | 1.67 | 0.60 |
| 1:H:250:TYR:OH | 1:H:266:LYS:NZ | 2.34 | 0.59 |
| 1:B:987:LEU:O | 1:B:991:LEU:HB2 | 2.02 | 0.59 |
| 1:F:971:ASP:OD1 | 1:F:973:SER:OG | 2.19 | 0.59 |
| 1:K:299:ASP:HB3 | 1:K:336:LYS:HB3 | 1.84 | 0.59 |
| 1:N:889:CYS:SG | 1:N:892:VAL:HG13 | 2.43 | 0.59 |
| 1:P:681:GLY:O | 1:P:685:SER:OG | 2.20 | 0.59 |
| 1:K:672:LEU:HB2 | 1:K:699:ALA:HB1 | 1.85 | 0.59 |
| 1:H:288:ARG:HH21 | 1:H:521:LEU:HA | 1.66 | 0.59 |
| 1:K:701:ALA:O | 1:K:725:THR:OG1 | 2.18 | 0.59 |
| 1:H:875:LEU:HB2 | 1:H:902:GLN:HG2 | 1.83 | 0.59 |
| 1:N:920:ARG:HA | 1:N:948:CYS:O | 2.03 | 0.59 |
| 1:B:824:GLU:HG2 | 1:B:852:ILE:HB | 1.84 | 0.59 |
| 1:K:888:TRP:HH2 | 1:F:507:ARG:HE | 1.50 | 0.59 |
| 1:H:921:ASP:OD1 | 1:H:950:SER:OG | 2.20 | 0.59 |
| 1:D:306:LYS:HD2 | 1:D:322:TRP:CE2 | 2.37 | 0.59 |
| 1:B:377:ARG:NH1 | 1:B:423:THR:O | 2.36 | 0.59 |
| 1:H:925:LYS:HA | 1:H:956:TYR:HE2 | 1.67 | 0.59 |
| 1:N:919:LEU:O | 1:N:948:CYS:N | 2.35 | 0.59 |
| 1:P:551:VAL:HG22 | 1:P:582:LYS:HG2 | 1.84 | 0.59 |
| 1:K:606:ALA:HB1 | 1:K:659:PHE:HE1 | 1.68 | 0.59 |
| 1:K:865:ASN:OD1 | 1:K:895:SER:OG | 2.21 | 0.58 |
| 1:P:858:ASN:HB2 | 1:P:887:PRO:HB3 | 1.85 | 0.58 |
| 1:H:716:THR:HG22 | 1:H:740:ASN:HD22 | 1.69 | 0.58 |
| 1:H:914:LEU:HB3 | 1:H:917:TRP:CG | 2.38 | 0.58 |
| 1:B:209:ARG:NH1 | 1:F:218:ASP:OD1 | 2.31 | 0.58 |
| 1:F:204:HIS:H | 1:F:219:GLN:HE22 | 1.51 | 0.58 |
| 1:P:983:LEU:C | 1:P:986:LYS:CB | 2.72 | 0.58 |
| 1:N:430:TYR:HA | 1:N:431:THR:OG1 | 2.03 | 0.58 |
| 1:D:588:SER:OG | 1:D:615:ASP:O | 2.16 | 0.58 |
| 1:L:174:GLY:N | 2:L:1101:ADP:O2B | 2.34 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:940:GLN:O | 1:F:968:VAL:N | 2.31 | 0.58 |
| 1:B:845:HIS:HA | 1:B:877:VAL:HG11 | 1.84 | 0.58 |
| 1:P:146:HIS:CE1 | 1:P:288:ARG:HD3 | 2.38 | 0.58 |
| 1:F:378:TYR:HD2 | 1:F:386:PHE:HD1 | 1.51 | 0.58 |
| 1:D:666:LEU:HB3 | 1:D:669:ILE:HD12 | 1.86 | 0.58 |
| 1:B:533:SEP:O3P | 1:B:665:THR:OG1 | 2.18 | 0.58 |
| 1:L:852:ILE:HG12 | 1:L:883:THR:HB | 1.85 | 0.58 |
| 1:F:535:GLN:O | 1:F:539:ASN:HB2 | 2.04 | 0.57 |
| 1:N:592:PRO:HD2 | 1:N:595:LEU:HD23 | 1.86 | 0.57 |
| 1:B:376:HIS:CD2 | 1:H:103:GLN:HG3 | 2.38 | 0.57 |
| 1:H:872:ILE:HA | 1:H:875:LEU:HG | 1.86 | 0.57 |
| 1:L:750:GLN:HG3 | 1:L:756:ILE:HD11 | 1.85 | 0.57 |
| 1:N:168:GLU:HB3 | 1:N:284:LEU:HD13 | 1.87 | 0.57 |
| 1:N:920:ARG:H | 1:N:923:GLU:HB2 | 1.68 | 0.57 |
| 1:D:588:SER:HB2 | 1:D:645:PRO:HG2 | 1.87 | 0.57 |
| 1:N:377:ARG:NH2 | 1:N:423:THR:O | 2.37 | 0.57 |
| 1:D:603:PRO:HA | 1:D:657:GLN:HE21 | 1.70 | 0.57 |
| 1:K:593:ASP:OD1 | 1:K:647:ARG:NH2 | 2.36 | 0.57 |
| 1:P:308:LEU:O | 1:P:312:VAL:HG22 | 2.05 | 0.57 |
| 1:D:475:ASN:HA | 1:D:508:HIS:CE1 | 2.40 | 0.57 |
| 1:K:745:ARG:HA | 1:K:772:ASP:HB3 | 1.86 | 0.57 |
| 1:N:927:LEU:O | 1:N:931:LEU:HB2 | 2.04 | 0.57 |
| 1:B:376:HIS:HD2 | 1:H:103:GLN:HG3 | 1.68 | 0.57 |
| 1:P:704:LEU:HD22 | 1:P:724:LEU:HD11 | 1.85 | 0.57 |
| 1:H:200:VAL:HG22 | 1:H:244:LEU:HB3 | 1.87 | 0.57 |
| 1:N:141:LYS:HB2 | 1:N:152:LEU:HD21 | 1.86 | 0.57 |
| 1:N:733:THR:O | 1:N:761:ASN:ND2 | 2.37 | 0.57 |
| 1:B:889:CYS:O | 1:B:892:VAL:HG22 | 2.05 | 0.57 |
| 1:F:743:ILE:HD11 | 1:F:746:LEU:HB2 | 1.86 | 0.56 |
| 1:K:592:PRO:HD2 | 1:K:595:LEU:HD22 | 1.85 | 0.56 |
| 1:B:230:PRO:HG3 | 1:F:256:GLN:HG2 | 1.86 | 0.56 |
| 1:P:205:LEU:HB3 | 1:P:253:PHE:HB2 | 1.86 | 0.56 |
| 1:K:588:SER:OG | 1:K:615:ASP:O | 2.20 | 0.56 |
| 1:N:245:PHE:HB2 | 1:N:275:VAL:HG12 | 1.87 | 0.56 |
| 1:B:192:ARG:HA | 1:B:195:LYS:HE3 | 1.86 | 0.56 |
| 1:D:249:GLY:H | 1:D:278:THR:HG22 | 1.70 | 0.56 |
| 1:P:817:GLU:HB3 | 1:P:818:GLU:HG3 | 1.87 | 0.56 |
| 1:L:344:THR:HG22 | 1:L:362:LEU:HD11 | 1.87 | 0.56 |
| 1:F:571:LEU:O | 1:F:574:GLU:HG2 | 2.05 | 0.56 |
| 1:N:308:LEU:O | 1:N:312:VAL:HG22 | 2.05 | 0.56 |
| 1:L:875:LEU:HB2 | 1:L:902:GLN:HG2 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:940:GLN:O | 1:K:968:VAL:N | 2.33 | 0.56 |
| 1:F:339:LEU:O | 1:F:342:VAL:HG22 | 2.06 | 0.56 |
| 1:N:668:ASP:OD2 | 1:N:696:ARG:NH1 | 2.38 | 0.56 |
| 1:N:967:LEU:HD21 | 1:N:970:PHE:HB3 | 1.86 | 0.56 |
| 1:L:756:ILE:HG22 | 1:L:783:LEU:HD13 | 1.86 | 0.56 |
| 1:D:174:GLY:N | 2:D:1101:ADP:O3B | 2.36 | 0.56 |
| 1:L:663:GLU:OE2 | 1:L:691:ARG:NH1 | 2.38 | 0.56 |
| 1:P:413:GLY:O | 1:P:414:SER:HB2 | 2.05 | 0.56 |
| 1:P:764:ASN:HA | 1:P:792:LYS:HD3 | 1.85 | 0.56 |
| 1:K:803:ASP:HB2 | 1:F:462:LYS:HA | 1.86 | 0.56 |
| 1:F:716:THR:HB | 1:F:740:ASN:HB2 | 1.86 | 0.56 |
| 1:D:308:LEU:O | 1:D:312:VAL:HG22 | 2.05 | 0.56 |
| 1:L:567:SER:HB2 | 1:L:571:LEU:HD23 | 1.88 | 0.56 |
| 1:F:868:LEU:HD11 | 1:F:886:LEU:HD22 | 1.88 | 0.56 |
| 1:B:921:ASP:OD1 | 1:B:950:SER:OG | 2.22 | 0.56 |
| 1:D:443:HIS:ND1 | 1:D:445:SER:OG | 2.37 | 0.56 |
| 1:D:434:ARG:HD3 | 1:D:438:THR:HB | 1.87 | 0.56 |
| 1:K:340:PHE:O | 1:K:344:THR:HG23 | 2.06 | 0.56 |
| 1:N:678:LYS:HE2 | 1:N:679:TYR:CE1 | 2.41 | 0.56 |
| 1:L:141:LYS:HB2 | 1:L:152:LEU:HD11 | 1.87 | 0.56 |
| 1:K:851:SER:HA | 1:K:881:LEU:HA | 1.88 | 0.56 |
| 1:P:983:LEU:C | 1:P:986:LYS:N | 2.58 | 0.56 |
| 1:N:140:TRP:HB3 | 1:N:148:ARG:HB3 | 1.88 | 0.56 |
| 1:K:360:THR:OG1 | 1:K:564:GLU:OE1 | 2.17 | 0.56 |
| 1:N:920:ARG:O | 1:N:924:ILE:N | 2.31 | 0.56 |
| 1:K:925:LYS:O | 1:K:929:GLU:HG3 | 2.05 | 0.56 |
| 1:B:532:GLU:OE2 | 1:B:533:SEP:N | 2.39 | 0.55 |
| 1:L:535:GLN:O | 1:L:539:ASN:HB2 | 2.06 | 0.55 |
| 1:H:325:ILE:HD13 | 1:H:331:LEU:HD13 | 1.86 | 0.55 |
| 1:P:344:THR:HG22 | 1:P:362:LEU:HD11 | 1.89 | 0.55 |
| 1:H:371:ILE:O | 1:H:375:SER:OG | 2.13 | 0.55 |
| 1:P:539:ASN:ND2 | 1:P:541:THR:O | 2.39 | 0.55 |
| 1:F:108:LEU:O | 1:F:111:SER:OG | 2.23 | 0.55 |
| 1:K:678:LYS:O | 1:K:682:LYS:HG2 | 2.06 | 0.55 |
| 1:D:816:SER:HB2 | 1:D:843:ASN:HB2 | 1.88 | 0.55 |
| 1:N:200:VAL:HG12 | 1:N:244:LEU:HB3 | 1.87 | 0.55 |
| 1:B:98:LEU:HD13 | 1:B:235:LEU:HD11 | 1.88 | 0.55 |
| 1:B:797:HIS:CD2 | 1:B:826:LYS:HB2 | 2.41 | 0.55 |
| 1:F:851:SER:HA | 1:F:881:LEU:HA | 1.89 | 0.55 |
| 1:K:720:GLU:HA | 1:K:744:HIS:HB2 | 1.89 | 0.55 |
| 1:K:830:CYS:O | 1:K:858:ASN:ND2 | 2.36 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:P:421:LEU:HB2 | 1:P:427:LEU:HD12 | 1.88 | 0.55 |
| 1:L:588:SER:HB2 | 1:L:645:PRO:HG2 | 1.89 | 0.55 |
| 1:F:192:ARG:O | 1:F:195:LYS:HG2 | 2.07 | 0.55 |
| 1:N:977:PHE:N | 1:N:977:PHE:CD1 | 2.75 | 0.55 |
| 1:P:983:LEU:O | 1:P:986:LYS:CB | 2.54 | 0.55 |
| 1:K:175:LYS:N | 2:K:1101:ADP:O3B | 2.40 | 0.55 |
| 1:K:621:THR:HG21 | 1:K:679:TYR:HD2 | 1.72 | 0.55 |
| 1:K:914:LEU:HB3 | 1:K:917:TRP:CG | 2.41 | 0.55 |
| 1:H:681:GLY:O | 1:H:685:SER:OG | 2.25 | 0.55 |
| 1:B:620:ALA:HB1 | 1:B:680:LEU:HD11 | 1.89 | 0.55 |
| 1:B:914:LEU:HB3 | 1:B:917:TRP:CG | 2.42 | 0.55 |
| 1:L:169:GLY:O | 1:L:280:THR:HA | 2.08 | 0.54 |
| 1:N:418:GLU:OE2 | 1:N:418:GLU:N | 2.40 | 0.54 |
| 1:N:824:GLU:HA | 1:N:852:ILE:HB | 1.89 | 0.54 |
| 1:F:588:SER:OG | 1:F:615:ASP:O | 2.18 | 0.54 |
| 1:H:889:CYS:O | 1:H:892:VAL:HG22 | 2.08 | 0.54 |
| 1:F:308:LEU:O | 1:F:312:VAL:HG22 | 2.08 | 0.54 |
| 1:L:896:LEU:HD12 | 1:L:923:GLU:HB3 | 1.88 | 0.54 |
| 1:H:421:LEU:HB2 | 1:H:427:LEU:HD12 | 1.90 | 0.54 |
| 1:P:665:THR:HB | 1:P:693:HIS:HB3 | 1.90 | 0.54 |
| 1:L:970:PHE:HE2 | 1:L:997:LEU:HD21 | 1.73 | 0.54 |
| 1:F:872:ILE:HA | 1:F:875:LEU:HG | 1.88 | 0.54 |
| 1:H:918:ARG:HB3 | 1:H:948:CYS:SG | 2.47 | 0.54 |
| 1:L:816:SER:HB2 | 1:L:843:ASN:HB2 | 1.90 | 0.54 |
| 1:K:889:CYS:O | 1:K:892:VAL:HG22 | 2.08 | 0.54 |
| 1:P:851:SER:HA | 1:P:881:LEU:HA | 1.88 | 0.54 |
| 1:H:816:SER:HB2 | 1:H:843:ASN:HB2 | 1.90 | 0.54 |
| 1:B:548:ALA:O | 1:B:552:ASN:ND2 | 2.41 | 0.53 |
| 1:D:776:ASN:H | 1:D:779:ASP:HB2 | 1.73 | 0.53 |
| 1:N:535:GLN:O | 1:N:539:ASN:HB2 | 2.09 | 0.53 |
| 1:D:463:GLU:HG3 | 1:F:774:ARG:NH2 | 2.23 | 0.53 |
| 1:P:666:LEU:HB3 | 1:P:669:ILE:HD12 | 1.89 | 0.53 |
| 1:B:552:ASN:ND2 | 1:B:583:SER:OG | 2.41 | 0.53 |
| 1:P:769:ILE:HG12 | 1:P:797:HIS:HB2 | 1.90 | 0.53 |
| 1:N:351:ARG:HG2 | 1:N:369:LEU:HD11 | 1.89 | 0.53 |
| 1:K:892:VAL:HG21 | 1:K:917:TRP:HA | 1.91 | 0.53 |
| 1:D:198:ARG:N | 1:D:242:GLU:O | 2.41 | 0.53 |
| 1:H:991:LEU:HD12 | 1:H:1019:PHE:CZ | 2.44 | 0.53 |
| 1:P:198:ARG:N | 1:P:242:GLU:O | 2.41 | 0.53 |
| 1:D:984:VAL:HG13 | 1:D:1015:ILE:HD11 | 1.90 | 0.53 |
| 1:P:406:PHE:CZ | 1:P:444:LYS:HE3 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:N:981:ALA:O | 1:N:984:VAL:N | 2.42 | 0.53 |
| 1:N:420:VAL:O | 1:N:424:ILE:HG13 | 2.08 | 0.53 |
| 1:H:962:GLU:HG3 | 1:H:990:VAL:HG13 | 1.90 | 0.53 |
| 1:F:677:ILE:HG23 | 1:F:707:VAL:HA | 1.90 | 0.53 |
| 1:N:941:GLN:HA | 1:N:967:LEU:HD11 | 1.91 | 0.53 |
| 1:N:997:LEU:O | 1:N:1019:PHE:HB3 | 2.08 | 0.53 |
| 1:D:595:LEU:HD12 | 1:D:651:LEU:HD11 | 1.91 | 0.53 |
| 1:H:830:CYS:O | 1:H:858:ASN:ND2 | 2.38 | 0.53 |
| 1:L:538:ARG:HD3 | 1:L:691:ARG:HD3 | 1.90 | 0.53 |
| 1:H:228:SER:OG | 1:H:231:THR:OG1 | 2.24 | 0.53 |
| 1:N:421:LEU:HB2 | 1:N:427:LEU:HD12 | 1.91 | 0.53 |
| 1:B:910:ALA:O | 1:B:940:GLN:N | 2.35 | 0.53 |
| 1:B:547:LYS:O | 1:B:551:VAL:HG23 | 2.09 | 0.53 |
| 1:N:656:LYS:C | 1:N:657:GLN:HE21 | 2.12 | 0.53 |
| 1:B:816:SER:HB2 | 1:B:843:ASN:CB | 2.39 | 0.53 |
| 1:H:321:LEU:O | 1:H:325:ILE:HG12 | 2.09 | 0.53 |
| 1:P:173:LYS:HE3 | 1:P:299:ASP:HA | 1.90 | 0.53 |
| 1:K:300:MET:N | 1:K:336:LYS:O | 2.36 | 0.53 |
| 1:L:108:LEU:O | 1:L:111:SER:OG | 2.26 | 0.53 |
| 1:N:108:LEU:O | 1:N:111:SER:OG | 2.27 | 0.53 |
| 1:H:209:ARG:NH1 | 1:L:218:ASP:OD1 | 2.33 | 0.53 |
| 1:N:321:LEU:O | 1:N:325:ILE:HG13 | 2.09 | 0.53 |
| 1:H:443:HIS:ND1 | 1:H:445:SER:OG | 2.41 | 0.53 |
| 1:B:673:ASN:H | 1:B:676:ASP:HB2 | 1.74 | 0.52 |
| 1:H:145:ARG:HE | 1:H:667:ARG:NH2 | 2.07 | 0.52 |
| 1:P:690:LEU:HD22 | 1:P:714:MET:HG3 | 1.89 | 0.52 |
| 1:D:845:HIS:HA | 1:D:877:VAL:HG11 | 1.91 | 0.52 |
| 1:L:865:ASN:OD1 | 1:L:895:SER:OG | 2.27 | 0.52 |
| 1:D:1019:PHE:HE2 | 1:D:1021:LEU:HD13 | 1.74 | 0.52 |
| 1:B:936:LEU:HB3 | 1:B:939:LEU:HB2 | 1.90 | 0.52 |
| 1:N:588:SER:OG | 1:N:615:ASP:O | 2.26 | 0.52 |
| 1:F:351:ARG:O | 1:F:352:GLN:HB2 | 2.09 | 0.52 |
| 1:P:824:GLU:HG2 | 1:P:852:ILE:HB | 1.92 | 0.52 |
| 1:K:674:LYS:O | 1:K:678:LYS:HG2 | 2.10 | 0.52 |
| 1:P:351:ARG:HD3 | 1:P:354:PHE:HB3 | 1.91 | 0.52 |
| 1:K:910:ALA:O | 1:K:940:GLN:N | 2.34 | 0.52 |
| 1:P:108:LEU:O | 1:P:111:SER:OG | 2.27 | 0.52 |
| 1:H:333:ASN:HA | 1:H:336:LYS:HZ2 | 1.73 | 0.52 |
| 1:L:493:TYR:O | 1:L:497:SER:OG | 2.25 | 0.52 |
| 1:L:889:CYS:O | 1:L:892:VAL:HG22 | 2.10 | 0.52 |
| 1:D:716:THR:HG23 | 1:D:740:ASN:HB2 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:K:987:LEU:HD22 | 1:K:1015:ILE:HD12 | 1.92 | 0.52 |
| 1:N:335:MET:HE3 | 1:N:341:VAL:HA | 1.91 | 0.52 |
| 1:H:588:SER:HB2 | 1:H:645:PRO:HD2 | 1.91 | 0.52 |
| 1:F:970:PHE:HE2 | 1:F:997:LEU:HD21 | 1.75 | 0.52 |
| 1:N:345:CYS:O | 1:N:349:MET:HG3 | 2.10 | 0.52 |
| 1:H:787:LEU:HD13 | 1:H:815:LEU:HD21 | 1.91 | 0.52 |
| 1:F:1015:ILE:HG23 | 1:F:1021:LEU:HD11 | 1.91 | 0.52 |
| 1:D:604:ASN:N | 1:D:604:ASN:OD1 | 2.43 | 0.52 |
| 1:D:325:ILE:HG12 | 1:D:331:LEU:HD23 | 1.90 | 0.52 |
| 1:B:749:GLN:HG2 | 1:B:774:ARG:NH2 | 2.24 | 0.52 |
| 1:L:499:THR:HG23 | 1:L:571:LEU:HD21 | 1.92 | 0.52 |
| 1:N:977:PHE:N | 1:N:977:PHE:HD1 | 2.06 | 0.52 |
| 1:P:857:GLU:HG3 | 1:P:915:LYS:HD3 | 1.90 | 0.52 |
| 1:F:988:SER:OG | 1:F:1014:ALA:O | 2.28 | 0.52 |
| 1:L:578:PHE:O | 1:L:582:LYS:NZ | 2.28 | 0.52 |
| 1:H:812:VAL:HG11 | 1:H:840:LEU:HB2 | 1.91 | 0.52 |
| 1:F:406:PHE:CZ | 1:F:444:LYS:HE3 | 2.44 | 0.52 |
| 1:H:1002:LEU:HD23 | 1:H:1007:PHE:CE2 | 2.44 | 0.52 |
| 1:L:443:HIS:ND1 | 1:L:445:SER:OG | 2.42 | 0.52 |
| 1:L:914:LEU:HB3 | 1:L:917:TRP:CG | 2.45 | 0.52 |
| 1:N:947:HIS:ND1 | 1:N:973:SER:O | 2.42 | 0.52 |
| 1:L:143:ASP:HB2 | 1:L:149:VAL:HG23 | 1.92 | 0.52 |
| 1:B:749:GLN:HG2 | 1:B:774:ARG:CZ | 2.40 | 0.52 |
| 1:P:299:ASP:HB3 | 1:P:336:LYS:HB3 | 1.92 | 0.52 |
| 1:B:145:ARG:HA | 1:B:523:VAL:HG22 | 1.90 | 0.52 |
| 1:F:921:ASP:OD1 | 1:F:950:SER:OG | 2.28 | 0.52 |
| 1:B:350:GLY:HA3 | 1:B:369:LEU:HD21 | 1.90 | 0.52 |
| 1:F:855:ILE:HG13 | 1:F:887:PRO:HD3 | 1.92 | 0.52 |
| 1:F:889:CYS:O | 1:F:892:VAL:HG22 | 2.10 | 0.52 |
| 1:L:228:SER:OG | 1:L:231:THR:OG1 | 2.24 | 0.52 |
| 1:F:875:LEU:HB2 | 1:F:902:GLN:HG2 | 1.91 | 0.51 |
| 1:H:228:SER:HG | 1:H:231:THR:HG1 | 1.58 | 0.51 |
| 1:K:986:LYS:O | 1:K:990:VAL:HG23 | 2.09 | 0.51 |
| 1:P:677:ILE:HG22 | 1:P:707:VAL:HG22 | 1.92 | 0.51 |
| 1:D:986:LYS:O | 1:D:990:VAL:HG23 | 2.10 | 0.51 |
| 1:B:420:VAL:O | 1:B:424:ILE:HG13 | 2.10 | 0.51 |
| 1:N:850:LEU:HD21 | 1:N:853:LEU:HD13 | 1.92 | 0.51 |
| 1:P:361:MET:O | 1:P:365:THR:OG1 | 2.23 | 0.51 |
| 1:P:345:CYS:O | 1:P:349:MET:HG3 | 2.11 | 0.51 |
| 1:H:142:LYS:HD2 | 1:H:168:GLU:OE2 | 2.11 | 0.51 |
| 1:N:859:TYR:CE1 | 1:N:889:CYS:HA | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:284:LEU:HG | 1:H:288:ARG:HG3 | 1.93 | 0.51 |
| 1:D:586:ILE:HG12 | 1:D:595:LEU:HD11 | 1.93 | 0.51 |
| 1:L:859:TYR:CE1 | 1:L:889:CYS:HA | 2.45 | 0.51 |
| 1:L:418:GLU:O | 1:L:422:VAL:HG23 | 2.10 | 0.51 |
| 1:B:308:LEU:O | 1:B:312:VAL:HG22 | 2.11 | 0.51 |
| 1:B:508:HIS:O | 1:B:511:MET:HG2 | 2.11 | 0.51 |
| 1:D:681:GLY:O | 1:D:685:SER:OG | 2.28 | 0.51 |
| 1:K:854:ASP:OD2 | 1:K:856:SER:OG | 2.22 | 0.51 |
| 1:B:788:ARG:NH1 | 1:B:817:GLU:OE2 | 2.44 | 0.51 |
| 1:B:312:VAL:O | 1:H:132:LYS:NZ | 2.44 | 0.51 |
| 1:L:97:ASP:HA | 1:L:100:VAL:HG12 | 1.93 | 0.51 |
| 1:P:499:THR:HA | 1:P:502:THR:HG22 | 1.93 | 0.51 |
| 1:P:696:ARG:HA | 1:P:721:ALA:HB3 | 1.92 | 0.51 |
| 1:B:604:ASN:N | 1:B:604:ASN:OD1 | 2.44 | 0.51 |
| 1:D:406:PHE:CZ | 1:D:444:LYS:HE3 | 2.45 | 0.51 |
| 1:B:225:ASP:HB2 | 1:F:405:LYS:NZ | 2.25 | 0.51 |
| 1:B:198:ARG:N | 1:B:242:GLU:O | 2.44 | 0.51 |
| 1:L:666:LEU:HB3 | 1:L:669:ILE:HD12 | 1.91 | 0.51 |
| 1:K:776:ASN:H | 1:K:779:ASP:HB2 | 1.75 | 0.51 |
| 1:K:134:PHE:CZ | 1:K:181:ARG:HG2 | 2.45 | 0.51 |
| 1:P:393:CYS:HB2 | 1:P:421:LEU:HD22 | 1.93 | 0.51 |
| 1:K:1015:ILE:HG22 | 1:K:1021:LEU:HD11 | 1.93 | 0.51 |
| 1:L:518:LEU:HD23 | 1:L:546:LEU:HB2 | 1.92 | 0.51 |
| 1:P:131:GLU:HG3 | 1:P:184:MET:HE1 | 1.93 | 0.51 |
| 1:L:308:LEU:O | 1:L:312:VAL:HG22 | 2.10 | 0.51 |
| 1:K:988:SER:OG | 1:K:1014:ALA:O | 2.29 | 0.51 |
| 1:N:285:ARG:NH1 | 1:N:484:THR:OG1 | 2.44 | 0.50 |
| 1:K:334:LEU:HD13 | 1:K:362:LEU:HD22 | 1.92 | 0.50 |
| 1:P:690:LEU:O | 1:P:715:HIS:N | 2.39 | 0.50 |
| 1:B:322:TRP:HA | 1:B:325:ILE:HD12 | 1.93 | 0.50 |
| 1:B:225:ASP:OD2 | 1:B:225:ASP:N | 2.30 | 0.50 |
| 1:H:480:ILE:HG12 | 1:H:515:HIS:HA | 1.94 | 0.50 |
| 1:N:968:VAL:HG12 | 1:N:998:GLN:HB2 | 1.92 | 0.50 |
| 1:L:769:ILE:HG12 | 1:L:797:HIS:HB2 | 1.93 | 0.50 |
| 1:N:547:LYS:O | 1:N:551:VAL:HG13 | 2.11 | 0.50 |
| 1:D:345:CYS:O | 1:D:349:MET:HG3 | 2.11 | 0.50 |
| 1:K:604:ASN:N | 1:K:604:ASN:OD1 | 2.42 | 0.50 |
| 1:P:135:THR:O | 2:P:1101:ADP:N6 | 2.43 | 0.50 |
| 1:F:986:LYS:O | 1:F:990:VAL:HG23 | 2.12 | 0.50 |
| 1:H:533:SEP:OG | 1:H:534:ILE:N | 2.41 | 0.50 |
| 1:D:889:CYS:O | 1:D:892:VAL:HG22 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:P:168:GLU:HB3 | 1:P:284:LEU:HD13 | 1.92 | 0.50 |
| 1:L:522:SER:O | 1:L:523:VAL:O | 2.30 | 0.50 |
| 1:N:914:LEU:HB3 | 1:N:917:TRP:CG | 2.47 | 0.50 |
| 1:H:852:ILE:HG12 | 1:H:883:THR:HB | 1.92 | 0.50 |
| 1:D:416:MET:HE3 | 1:N:420:VAL:HG22 | 1.92 | 0.50 |
| 1:H:578:PHE:O | 1:H:582:LYS:NZ | 2.26 | 0.50 |
| 1:D:940:GLN:O | 1:D:968:VAL:N | 2.34 | 0.50 |
| 1:D:756:ILE:HD11 | 1:D:779:ASP:HB3 | 1.92 | 0.50 |
| 1:K:535:GLN:O | 1:K:539:ASN:HB2 | 2.11 | 0.50 |
| 1:K:903:LEU:HD21 | 1:K:909:LEU:HD12 | 1.93 | 0.50 |
| 1:L:986:LYS:O | 1:L:990:VAL:HG23 | 2.12 | 0.50 |
| 1:H:568:LYS:HD3 | 1:H:601:TYR:CZ | 2.46 | 0.50 |
| 1:K:862:LYS:NZ | 1:F:574:GLU:OE2 | 2.35 | 0.50 |
| 1:B:206:ARG:HG2 | 1:B:207:SER:N | 2.26 | 0.50 |
| 1:D:266:LYS:HG3 | 1:D:290:VAL:HG21 | 1.94 | 0.50 |
| 1:D:474:LEU:HD23 | 1:D:477:MET:HE3 | 1.94 | 0.50 |
| 1:N:672:LEU:HB2 | 1:N:699:ALA:HB1 | 1.92 | 0.50 |
| 1:P:661:THR:HG23 | 1:P:689:ASN:HB3 | 1.94 | 0.50 |
| 1:D:108:LEU:O | 1:D:111:SER:OG | 2.29 | 0.50 |
| 1:F:911:LYS:HG2 | 1:F:941:GLN:HG2 | 1.94 | 0.50 |
| 1:N:582:LYS:O | 1:N:610:ASP:N | 2.44 | 0.50 |
| 1:H:503:ARG:HG3 | 1:H:571:LEU:HD11 | 1.94 | 0.50 |
| 1:L:146:HIS:CE1 | 1:L:288:ARG:HE | 2.29 | 0.50 |
| 1:P:420:VAL:O | 1:P:424:ILE:HG13 | 2.12 | 0.50 |
| 1:D:228:SER:OG | 1:D:231:THR:OG1 | 2.26 | 0.50 |
| 1:N:974:THR:C | 1:N:975:GLU:OE2 | 2.51 | 0.50 |
| 1:K:816:SER:HA | 1:K:847:LEU:HD21 | 1.93 | 0.50 |
| 1:D:663:GLU:OE2 | 1:D:691:ARG:NH1 | 2.44 | 0.50 |
| 1:B:1003:THR:HG23 | 1:B:1024:ALA:HA | 1.93 | 0.50 |
| 1:P:103:GLN:OE1 | 1:P:103:GLN:HA | 2.10 | 0.50 |
| 1:D:824:GLU:HG2 | 1:D:852:ILE:HB | 1.93 | 0.49 |
| 1:N:970:PHE:HE2 | 1:N:997:LEU:HD21 | 1.76 | 0.49 |
| 1:D:599:PHE:CD1 | 1:D:651:LEU:HD22 | 2.47 | 0.49 |
| 1:F:925:LYS:O | 1:F:929:GLU:HG3 | 2.12 | 0.49 |
| 1:H:547:LYS:O | 1:H:551:VAL:HG12 | 2.12 | 0.49 |
| 1:P:893:HIS:HB2 | 1:P:923:GLU:HG2 | 1.92 | 0.49 |
| 1:P:923:GLU:N | 1:P:923:GLU:OE1 | 2.45 | 0.49 |
| 1:H:269:HIS:NE2 | 1:H:1017:GLY:HA2 | 2.27 | 0.49 |
| 1:K:799:THR:HG22 | 1:K:828:VAL:HG22 | 1.94 | 0.49 |
| 1:H:776:ASN:H | 1:H:779:ASP:HB2 | 1.77 | 0.49 |
| 1:B:406:PHE:CZ | 1:B:444:LYS:HE3 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:811:ILE:O | 1:L:815:LEU:HG | 2.12 | 0.49 |
| 1:H:418:GLU:O | 1:H:422:VAL:HG23 | 2.12 | 0.49 |
| 1:D:515:HIS:NE2 | 1:D:547:LYS:HD2 | 2.27 | 0.49 |
| 1:F:769:ILE:HG12 | 1:F:797:HIS:HB2 | 1.94 | 0.49 |
| 1:P:355:GLN:HG2 | 1:P:357:HIS:CE1 | 2.48 | 0.49 |
| 1:B:474:LEU:HD23 | 1:B:477:MET:HE3 | 1.94 | 0.49 |
| 1:L:621:THR:HG1 | 1:L:645:PRO:N | 2.10 | 0.49 |
| 1:N:306:LYS:HD2 | 1:N:322:TRP:CE2 | 2.48 | 0.49 |
| 1:D:661:THR:HG23 | 1:D:689:ASN:HB3 | 1.93 | 0.49 |
| 1:P:335:MET:HE3 | 1:P:341:VAL:HA | 1.94 | 0.49 |
| 1:K:552:ASN:ND2 | 1:K:585:TYR:HB2 | 2.28 | 0.49 |
| 1:K:335:MET:HG3 | 1:K:341:VAL:HG22 | 1.93 | 0.49 |
| 1:H:518:LEU:HD21 | 1:H:547:LYS:HG2 | 1.93 | 0.49 |
| 1:D:1006:GLU:O | 1:D:1007:PHE:HB2 | 2.13 | 0.49 |
| 1:P:868:LEU:HD11 | 1:P:886:LEU:HG | 1.95 | 0.49 |
| 1:F:492:LEU:HG | 1:F:564:GLU:HG3 | 1.93 | 0.49 |
| 1:N:474:LEU:HD23 | 1:N:477:MET:HE3 | 1.93 | 0.49 |
| 1:H:859:TYR:CE1 | 1:H:889:CYS:HA | 2.47 | 0.49 |
| 1:H:333:ASN:OD1 | 1:H:336:LYS:NZ | 2.37 | 0.49 |
| 1:D:743:ILE:HG21 | 1:D:746:LEU:HD22 | 1.93 | 0.49 |
| 1:F:393:CYS:HB2 | 1:F:421:LEU:HD22 | 1.93 | 0.49 |
| 1:H:474:LEU:HD23 | 1:H:477:MET:HE3 | 1.94 | 0.49 |
| 1:H:984:VAL:HG22 | 1:H:1007:PHE:HE1 | 1.78 | 0.49 |
| 1:F:672:LEU:HD12 | 1:F:677:ILE:HG13 | 1.94 | 0.49 |
| 1:N:653:PHE:HE2 | 1:N:679:TYR:CD1 | 2.30 | 0.49 |
| 1:K:900:LEU:HG | 1:K:930:PHE:CG | 2.48 | 0.49 |
| 1:B:752:PRO:HA | 1:B:757:ASP:OD1 | 2.13 | 0.49 |
| 1:H:471:ASN:O | 1:H:475:ASN:HB2 | 2.12 | 0.49 |
| 1:D:886:LEU:HD12 | 1:D:917:TRP:HZ2 | 1.77 | 0.49 |
| 1:B:174:GLY:N | 2:B:1101:ADP:O2B | 2.44 | 0.49 |
| 1:P:698:ALA:HA | 1:P:723:PRO:HD3 | 1.94 | 0.49 |
| 1:H:335:MET:HE3 | 1:H:341:VAL:HA | 1.94 | 0.49 |
| 1:K:673:ASN:O | 1:K:677:ILE:HG13 | 2.12 | 0.49 |
| 1:D:324:GLN:NE2 | 1:D:354:PHE:O | 2.46 | 0.49 |
| 1:B:340:PHE:O | 1:B:344:THR:HG22 | 2.11 | 0.49 |
| 1:F:405:LYS:HE3 | 1:F:407:ASP:O | 2.13 | 0.49 |
| 1:P:750:GLN:HG3 | 1:P:756:ILE:HD11 | 1.95 | 0.49 |
| 1:H:334:LEU:HD13 | 1:H:362:LEU:HD22 | 1.95 | 0.49 |
| 1:B:430:TYR:HD2 | 1:B:438:THR:HB | 1.78 | 0.49 |
| 1:H:604:ASN:N | 1:H:604:ASN:OD1 | 2.46 | 0.49 |
| 1:L:420:VAL:O | 1:L:424:ILE:HG13 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:916:ASN:HA | 1:P:946:GLY:HA3 | 1.94 | 0.49 |
| 1:B:665:THR:HG23 | 1:B:693:HIS:HB3 | 1.95 | 0.49 |
| 1:H:715:HIS:CE1 | 1:H:739:GLN:HE21 | 2.30 | 0.49 |
| 1:N:480:ILE:HD12 | 1:N:554:PHE:HB2 | 1.93 | 0.49 |
| 1:P:169:GLY:O | 1:P:280:THR:HA | 2.13 | 0.49 |
| 1:P:910:ALA:O | 1:P:940:GLN:N | 2.35 | 0.49 |
| 1:N:788:ARG:NH2 | 1:N:817:GLU:OE1 | 2.45 | 0.48 |
| 1:B:691:ARG:HG2 | 1:B:715:HIS:HB3 | 1.95 | 0.48 |
| 1:B:267:GLU:OE1 | 1:B:270:ARG:NH1 | 2.46 | 0.48 |
| 1:L:900:LEU:O | 1:L:904:GLU:HG3 | 2.13 | 0.48 |
| 1:K:547:LYS:O | 1:K:551:VAL:HG23 | 2.12 | 0.48 |
| 1:D:932:GLU:HG3 | 1:D:960:VAL:HG13 | 1.95 | 0.48 |
| 1:H:535:GLN:O | 1:H:539:ASN:HB2 | 2.13 | 0.48 |
| 1:D:235:LEU:HD23 | 1:D:239:LEU:HD23 | 1.95 | 0.48 |
| 1:D:98:LEU:HD11 | 1:D:239:LEU:HD21 | 1.94 | 0.48 |
| 1:D:145:ARG:HA | 1:D:523:VAL:HG22 | 1.94 | 0.48 |
| 1:B:529:TRP:HA | 1:B:529:TRP:CE3 | 2.47 | 0.48 |
| 1:H:788:ARG:HG3 | 1:H:788:ARG:HH21 | 1.78 | 0.48 |
| 1:K:385:ASP:HB3 | 1:K:388:ARG:HB2 | 1.94 | 0.48 |
| 1:F:825:MET:HG2 | 1:F:827:LEU:HD13 | 1.96 | 0.48 |
| 1:L:464:PRO:HA | 1:L:467:VAL:HG12 | 1.94 | 0.48 |
| 1:N:918:ARG:O | 1:N:920:ARG:NH1 | 2.47 | 0.48 |
| 1:N:940:GLN:O | 1:N:941:GLN:HB3 | 2.14 | 0.48 |
| 1:L:588:SER:OG | 1:L:615:ASP:O | 2.23 | 0.48 |
| 1:B:96:GLU:O | 1:B:100:VAL:HG13 | 2.13 | 0.48 |
| 1:P:306:LYS:HD2 | 1:P:322:TRP:CE2 | 2.48 | 0.48 |
| 1:K:339:LEU:O | 1:K:343:ILE:HG13 | 2.14 | 0.48 |
| 1:L:92:GLN:O | 1:L:93:VAL:HG13 | 2.14 | 0.48 |
| 1:N:918:ARG:HB3 | 1:N:918:ARG:HE | 1.38 | 0.48 |
| 1:K:306:LYS:HD3 | 1:K:322:TRP:CE2 | 2.49 | 0.48 |
| 1:N:888:TRP:HA | 1:N:892:VAL:HG11 | 1.94 | 0.48 |
| 1:N:599:PHE:HB3 | 1:N:657:GLN:OE1 | 2.13 | 0.48 |
| 1:P:893:HIS:CD2 | 1:P:918:ARG:HB2 | 2.49 | 0.48 |
| 1:P:571:LEU:HD22 | 1:P:574:GLU:HG3 | 1.96 | 0.48 |
| 1:K:893:HIS:HB2 | 1:K:923:GLU:HG2 | 1.95 | 0.48 |
| 1:P:676:ASP:O | 1:P:680:LEU:HD13 | 2.14 | 0.48 |
| 1:N:690:LEU:HD23 | 1:N:714:MET:SD | 2.53 | 0.48 |
| 1:F:97:ASP:HA | 1:F:100:VAL:HG12 | 1.96 | 0.48 |
| 1:P:163:SER:HB2 | 1:P:274:MET:CE | 2.44 | 0.48 |
| 1:K:888:TRP:HA | 1:K:892:VAL:HG11 | 1.95 | 0.48 |
| 1:F:166:LEU:HD22 | 1:F:287:ILE:HD12 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:420:VAL:O | 1:H:424:ILE:HG13 | 2.14 | 0.48 |
| 1:L:198:ARG:N | 1:L:242:GLU:O | 2.46 | 0.48 |
| 1:F:562:PHE:O | 1:F:565:SER:OG | 2.27 | 0.48 |
| 1:B:533:SEP:OG | 1:B:534:ILE:N | 2.47 | 0.48 |
| 1:F:889:CYS:SG | 1:F:892:VAL:HG13 | 2.53 | 0.48 |
| 1:K:525:LYS:HE3 | 1:K:525:LYS:HB2 | 1.46 | 0.48 |
| 1:N:860:LEU:HB2 | 1:N:864:GLY:HA3 | 1.95 | 0.48 |
| 1:K:1002:LEU:O | 1:K:1023:THR:HA | 2.13 | 0.48 |
| 1:L:285:ARG:O | 1:L:520:GLY:HA3 | 2.13 | 0.48 |
| 1:F:663:GLU:HG3 | 1:F:691:ARG:HB2 | 1.95 | 0.48 |
| 1:D:889:CYS:SG | 1:D:892:VAL:HG13 | 2.54 | 0.48 |
| 1:N:967:LEU:HD11 | 1:N:969:PHE:O | 2.13 | 0.48 |
| 1:F:360:THR:OG1 | 1:F:564:GLU:OE1 | 2.20 | 0.48 |
| 1:H:645:PRO:O | 1:H:649:VAL:HG23 | 2.14 | 0.47 |
| 1:B:925:LYS:HA | 1:B:956:TYR:CE2 | 2.46 | 0.47 |
| 1:K:665:THR:HG23 | 1:K:693:HIS:HB3 | 1.95 | 0.47 |
| 1:L:925:LYS:HB2 | 1:L:925:LYS:HE2 | 1.71 | 0.47 |
| 1:L:421:LEU:HB2 | 1:L:427:LEU:HD12 | 1.95 | 0.47 |
| 1:P:93:VAL:HG11 | 1:P:235:LEU:HD13 | 1.96 | 0.47 |
| 1:N:593:ASP:OD1 | 1:N:647:ARG:NH2 | 2.42 | 0.47 |
| 1:K:828:VAL:C | 1:K:830:CYS:H | 2.16 | 0.47 |
| 1:P:479:SER:O | 1:P:483:ILE:HG13 | 2.14 | 0.47 |
| 1:H:412:HIS:HE1 | 1:H:436:LYS:HG2 | 1.79 | 0.47 |
| 1:K:205:LEU:HB2 | 1:K:248:ASP:O | 2.13 | 0.47 |
| 1:F:852:ILE:HG12 | 1:F:883:THR:HB | 1.95 | 0.47 |
| 1:N:851:SER:HA | 1:N:881:LEU:HA | 1.97 | 0.47 |
| 1:P:955:LEU:HD12 | 1:P:983:LEU:CA | 2.43 | 0.47 |
| 1:D:886:LEU:HD12 | 1:D:917:TRP:CZ2 | 2.50 | 0.47 |
| 1:L:824:GLU:HG2 | 1:L:852:ILE:HD12 | 1.96 | 0.47 |
| 1:H:360:THR:OG1 | 1:H:564:GLU:OE1 | 2.25 | 0.47 |
| 1:B:967:LEU:O | 1:B:997:LEU:HD12 | 2.14 | 0.47 |
| 1:P:888:TRP:HA | 1:P:892:VAL:HG11 | 1.96 | 0.47 |
| 1:F:666:LEU:HB3 | 1:F:669:ILE:HD12 | 1.97 | 0.47 |
| 1:L:745:ARG:HA | 1:L:772:ASP:HB3 | 1.95 | 0.47 |
| 1:L:406:PHE:CZ | 1:L:444:LYS:HE3 | 2.49 | 0.47 |
| 1:H:168:GLU:HB3 | 1:H:284:LEU:HD13 | 1.96 | 0.47 |
| 1:F:240:HIS:CE1 | 1:F:241:LYS:HG3 | 2.49 | 0.47 |
| 1:L:306:LYS:HD2 | 1:L:322:TRP:CE2 | 2.48 | 0.47 |
| 1:L:924:ILE:HA | 1:L:924:ILE:HD13 | 1.67 | 0.47 |
| 1:H:947:HIS:HD2 | 1:H:949:VAL:HB | 1.80 | 0.47 |
| 1:D:827:LEU:HD23 | 1:D:832:LEU:HD11 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:N:740:ASN:HD22 | 1:N:767:ARG:HB2 | 1.79 | 0.47 |
| 1:H:571:LEU:O | 1:H:574:GLU:HG2 | 2.15 | 0.47 |
| 1:D:461:SER:O | 1:F:802:SER:OG | 2.33 | 0.47 |
| 1:H:851:SER:HA | 1:H:881:LEU:HA | 1.95 | 0.47 |
| 1:D:306:LYS:HD2 | 1:D:322:TRP:CD2 | 2.50 | 0.47 |
| 1:B:889:CYS:SG | 1:B:892:VAL:HG13 | 2.55 | 0.47 |
| 1:K:962:GLU:HG3 | 1:K:990:VAL:HG22 | 1.96 | 0.47 |
| 1:P:321:LEU:O | 1:P:325:ILE:HG13 | 2.14 | 0.47 |
| 1:N:739:GLN:O | 1:N:740:ASN:ND2 | 2.47 | 0.47 |
| 1:P:663:GLU:HG3 | 1:P:691:ARG:HB2 | 1.95 | 0.47 |
| 1:N:898:LYS:HB3 | 1:N:898:LYS:HE3 | 1.74 | 0.47 |
| 1:H:901:LYS:HA | 1:H:901:LYS:HD3 | 1.67 | 0.47 |
| 1:H:1003:THR:HG22 | 1:H:1024:ALA:HB3 | 1.96 | 0.47 |
| 1:L:509:LEU:O | 1:L:512:VAL:HG22 | 2.15 | 0.47 |
| 1:D:288:ARG:NH1 | 1:D:520:GLY:O | 2.48 | 0.47 |
| 1:F:746:LEU:HD12 | 1:F:746:LEU:HA | 1.76 | 0.47 |
| 1:B:224:PRO:HB2 | 1:B:227:ILE:HG13 | 1.95 | 0.47 |
| 1:H:205:LEU:HB3 | 1:H:253:PHE:HB2 | 1.96 | 0.47 |
| 1:D:664:VAL:HG22 | 1:D:692:LEU:HD23 | 1.97 | 0.47 |
| 1:N:759:LEU:HD12 | 1:N:759:LEU:HA | 1.68 | 0.47 |
| 1:P:914:LEU:HD12 | 1:P:917:TRP:CZ2 | 2.50 | 0.47 |
| 1:P:324:GLN:NE2 | 1:P:354:PHE:H | 2.09 | 0.47 |
| 1:B:93:VAL:HG22 | 1:B:231:THR:HG23 | 1.97 | 0.47 |
| 1:N:139:MET:HB2 | 1:N:152:LEU:HB2 | 1.96 | 0.47 |
| 1:L:499:THR:HA | 1:L:502:THR:HG22 | 1.97 | 0.47 |
| 1:F:420:VAL:O | 1:F:424:ILE:HG13 | 2.14 | 0.47 |
| 1:F:532:GLU:HG3 | 1:F:718:MET:HE1 | 1.97 | 0.47 |
| 1:N:145:ARG:HD2 | 1:N:667:ARG:CZ | 2.45 | 0.47 |
| 1:N:664:VAL:HG22 | 1:N:692:LEU:HD23 | 1.96 | 0.47 |
| 1:L:824:GLU:HG2 | 1:L:852:ILE:HB | 1.97 | 0.47 |
| 1:L:479:SER:O | 1:L:483:ILE:HG13 | 2.15 | 0.47 |
| 1:N:269:HIS:CD2 | 1:N:1017:GLY:HA2 | 2.51 | 0.47 |
| 1:D:214:GLU:N | 1:D:214:GLU:OE1 | 2.46 | 0.47 |
| 1:F:770:LEU:HB2 | 1:F:798:LEU:HD23 | 1.96 | 0.46 |
| 1:N:418:GLU:O | 1:N:422:VAL:HG23 | 2.15 | 0.46 |
| 1:P:701:ALA:HB2 | 1:P:723:PRO:HG2 | 1.95 | 0.46 |
| 1:K:533:SEP:O1P | 1:K:613:LYS:NZ | 2.35 | 0.46 |
| 1:H:401:VAL:HG11 | 1:H:490:LEU:HD22 | 1.96 | 0.46 |
| 1:P:744:HIS:ND1 | 1:P:771:ASP:OD2 | 2.42 | 0.46 |
| 1:L:145:ARG:HG2 | 1:L:523:VAL:HB | 1.96 | 0.46 |
| 1:B:826:LYS:HG2 | 1:B:854:ASP:HB3 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:655:TRP:HB2 | 1:N:657:GLN:HE22 | 1.80 | 0.46 |
| 1:L:161:LEU:HD11 | 1:L:276:ILE:HD11 | 1.98 | 0.46 |
| 1:L:321:LEU:O | 1:L:325:ILE:HG13 | 2.14 | 0.46 |
| 1:B:666:LEU:HB3 | 1:B:669:ILE:HD12 | 1.95 | 0.46 |
| 1:D:330:CYS:HB3 | 1:D:357:HIS:O | 2.15 | 0.46 |
| 1:P:931:LEU:HD23 | 1:P:931:LEU:HA | 1.83 | 0.46 |
| 1:L:145:ARG:CG | 1:L:523:VAL:HB | 2.45 | 0.46 |
| 1:K:552:ASN:HD22 | 1:K:585:TYR:HB2 | 1.79 | 0.46 |
| 1:L:571:LEU:O | 1:L:574:GLU:HG2 | 2.14 | 0.46 |
| 1:H:889:CYS:SG | 1:H:892:VAL:HG13 | 2.54 | 0.46 |
| 1:K:923:GLU:N | 1:K:923:GLU:OE1 | 2.49 | 0.46 |
| 1:P:708:LEU:O | 1:P:731:TYR:OH | 2.33 | 0.46 |
| 1:H:954:TRP:O | 1:H:958:MET:HG2 | 2.15 | 0.46 |
| 1:P:670:ASN:O | 1:P:699:ALA:HB2 | 2.15 | 0.46 |
| 1:F:923:GLU:OE1 | 1:F:923:GLU:N | 2.49 | 0.46 |
| 1:N:181:ARG:O | 1:N:184:MET:HG3 | 2.15 | 0.46 |
| 1:H:104:ASN:HB3 | 1:H:222:ASN:HB2 | 1.97 | 0.46 |
| 1:F:493:TYR:O | 1:F:497:SER:OG | 2.30 | 0.46 |
| 1:P:694:ILE:HG21 | 1:P:700:MET:HG2 | 1.97 | 0.46 |
| 1:K:365:THR:O | 1:K:369:LEU:HB2 | 2.16 | 0.46 |
| 1:F:990:VAL:O | 1:F:994:LEU:HG | 2.16 | 0.46 |
| 1:B:532:GLU:H | 1:B:536:SER:CB | 2.29 | 0.46 |
| 1:K:145:ARG:HA | 1:K:523:VAL:HG22 | 1.98 | 0.46 |
| 1:K:267:GLU:OE1 | 1:K:270:ARG:NH1 | 2.48 | 0.46 |
| 1:K:285:ARG:O | 1:K:520:GLY:HA3 | 2.15 | 0.46 |
| 1:F:471:ASN:O | 1:F:475:ASN:ND2 | 2.34 | 0.46 |
| 1:L:664:VAL:HG22 | 1:L:692:LEU:HD23 | 1.97 | 0.46 |
| 1:B:538:ARG:HD3 | 1:B:716:THR:HG21 | 1.97 | 0.46 |
| 1:K:142:LYS:HD2 | 1:K:168:GLU:OE2 | 2.15 | 0.46 |
| 1:D:347:ILE:O | 1:D:351:ARG:HB2 | 2.16 | 0.46 |
| 1:L:991:LEU:HD23 | 1:L:1019:PHE:HZ | 1.80 | 0.46 |
| 1:B:860:LEU:HD11 | 1:B:887:PRO:HG2 | 1.97 | 0.46 |
| 1:B:954:TRP:O | 1:B:958:MET:HG2 | 2.16 | 0.46 |
| 1:N:568:LYS:HD3 | 1:N:601:TYR:CZ | 2.51 | 0.46 |
| 1:K:406:PHE:CZ | 1:K:444:LYS:HE3 | 2.51 | 0.46 |
| 1:L:690:LEU:HD23 | 1:L:714:MET:HG3 | 1.98 | 0.46 |
| 1:P:974:THR:HG23 | 1:P:975:GLU:N | 2.30 | 0.46 |
| 1:K:914:LEU:HB3 | 1:K:917:TRP:CD2 | 2.51 | 0.46 |
| 1:P:552:ASN:OD1 | 1:P:583:SER:OG | 2.33 | 0.46 |
| 1:B:932:GLU:HG3 | 1:B:960:VAL:HG13 | 1.96 | 0.46 |
| 1:K:743:ILE:HD13 | 1:K:746:LEU:HD22 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:367:TYR:O | 1:F:371:ILE:HG12 | 2.15 | 0.46 |
| 1:K:666:LEU:HB3 | 1:K:669:ILE:HD12 | 1.97 | 0.46 |
| 1:L:743:ILE:HD12 | 1:L:746:LEU:HD22 | 1.96 | 0.46 |
| 1:D:421:LEU:HB2 | 1:D:427:LEU:HD12 | 1.98 | 0.46 |
| 1:F:816:SER:HB2 | 1:F:843:ASN:HB2 | 1.96 | 0.46 |
| 1:D:285:ARG:NH1 | 1:D:517:SER:O | 2.49 | 0.46 |
| 1:N:911:LYS:HG2 | 1:N:941:GLN:HG2 | 1.96 | 0.46 |
| 1:H:406:PHE:CZ | 1:H:444:LYS:HE3 | 2.51 | 0.46 |
| 1:H:990:VAL:O | 1:H:994:LEU:HG | 2.16 | 0.46 |
| 1:B:132:LYS:NZ | 1:H:312:VAL:O | 2.49 | 0.46 |
| 1:F:787:LEU:HD13 | 1:F:815:LEU:HD21 | 1.97 | 0.46 |
| 1:D:823:GLN:HA | 1:D:850:LEU:HA | 1.97 | 0.46 |
| 1:D:872:ILE:O | 1:D:902:GLN:HG3 | 2.15 | 0.46 |
| 1:H:716:THR:CG2 | 1:H:740:ASN:HD22 | 2.28 | 0.46 |
| 1:L:168:GLU:HA | 1:L:279:THR:O | 2.16 | 0.46 |
| 1:L:955:LEU:HD13 | 1:L:983:LEU:HA | 1.98 | 0.46 |
| 1:H:175:LYS:O | 1:H:178:LEU:HB3 | 2.15 | 0.46 |
| 1:P:166:LEU:HD22 | 1:P:287:ILE:HD12 | 1.98 | 0.46 |
| 1:N:173:LYS:HA | 1:N:173:LYS:HD3 | 1.76 | 0.46 |
| 1:F:284:LEU:HG | 1:F:288:ARG:HG3 | 1.96 | 0.46 |
| 1:N:970:PHE:CZ | 1:N:1000:VAL:HG13 | 2.50 | 0.46 |
| 1:P:378:TYR:HD1 | 1:P:386:PHE:HD1 | 1.63 | 0.46 |
| 1:F:645:PRO:HA | 1:F:646:PRO:HD3 | 1.87 | 0.45 |
| 1:N:595:LEU:HA | 1:N:595:LEU:HD13 | 1.76 | 0.45 |
| 1:K:588:SER:HB2 | 1:K:645:PRO:HD2 | 1.97 | 0.45 |
| 1:N:511:MET:HG2 | 1:P:891:ASP:OD2 | 2.16 | 0.45 |
| 1:L:911:LYS:HG2 | 1:L:941:GLN:HG2 | 1.98 | 0.45 |
| 1:B:108:LEU:O | 1:B:111:SER:OG | 2.33 | 0.45 |
| 1:N:456:SER:OG | 1:N:498:SER:HB3 | 2.16 | 0.45 |
| 1:K:288:ARG:HH11 | 1:K:288:ARG:HG2 | 1.81 | 0.45 |
| 1:L:518:LEU:HD21 | 1:L:547:LYS:HG2 | 1.99 | 0.45 |
| 1:P:355:GLN:HG2 | 1:P:357:HIS:HE1 | 1.81 | 0.45 |
| 1:H:206:ARG:NH2 | 1:H:406:PHE:O | 2.48 | 0.45 |
| 1:H:359:GLN:NE2 | 1:H:493:TYR:OH | 2.42 | 0.45 |
| 1:P:496:GLY:HA2 | 1:P:564:GLU:O | 2.16 | 0.45 |
| 1:K:991:LEU:HD23 | 1:K:1019:PHE:HZ | 1.81 | 0.45 |
| 1:K:164:PRO:HG2 | 1:K:290:VAL:CG1 | 2.46 | 0.45 |
| 1:B:730:GLN:HG2 | 1:B:753:GLY:O | 2.16 | 0.45 |
| 1:H:557:CYS:O | 1:H:561:LEU:HD13 | 2.16 | 0.45 |
| 1:B:526:ARG:C | 1:B:526:ARG:HD2 | 2.35 | 0.45 |
| 1:P:502:THR:HG21 | 1:P:565:SER:HB2 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:284:LEU:HG | 1:L:288:ARG:HG3 | 1.98 | 0.45 |
| 1:L:649:VAL:O | 1:L:653:PHE:HB2 | 2.17 | 0.45 |
| 1:D:900:LEU:O | 1:D:904:GLU:HG3 | 2.16 | 0.45 |
| 1:L:333:ASN:ND2 | 1:L:593:ASP:OD1 | 2.46 | 0.45 |
| 1:P:855:ILE:HG13 | 1:P:887:PRO:HD3 | 1.98 | 0.45 |
| 1:N:910:ALA:O | 1:N:940:GLN:N | 2.45 | 0.45 |
| 1:D:343:ILE:O | 1:D:347:ILE:HG13 | 2.16 | 0.45 |
| 1:D:752:PRO:HA | 1:D:757:ASP:OD1 | 2.17 | 0.45 |
| 1:F:145:ARG:CZ | 1:F:523:VAL:HG21 | 2.47 | 0.45 |
| 1:P:267:GLU:HB3 | 1:P:269:HIS:CE1 | 2.52 | 0.45 |
| 1:N:285:ARG:O | 1:N:520:GLY:HA3 | 2.15 | 0.45 |
| 1:D:816:SER:HB2 | 1:D:843:ASN:CB | 2.46 | 0.45 |
| 1:K:889:CYS:SG | 1:K:892:VAL:HG13 | 2.57 | 0.45 |
| 1:F:240:HIS:CG | 1:F:241:LYS:H | 2.34 | 0.45 |
| 1:K:443:HIS:ND1 | 1:K:445:SER:OG | 2.48 | 0.45 |
| 1:D:371:ILE:HD12 | 1:D:426:LEU:HD21 | 1.98 | 0.45 |
| 1:F:335:MET:HG3 | 1:F:341:VAL:HG22 | 1.98 | 0.45 |
| 1:H:337:THR:HA | 1:H:338:PRO:HD3 | 1.76 | 0.45 |
| 1:H:141:LYS:HB2 | 1:H:152:LEU:HD11 | 1.99 | 0.45 |
| 1:K:578:PHE:O | 1:K:582:LYS:NZ | 2.32 | 0.45 |
| 1:F:978:LEU:HD22 | 1:F:1006:GLU:HB2 | 1.99 | 0.45 |
| 1:F:924:ILE:HD12 | 1:F:924:ILE:HA | 1.69 | 0.45 |
| 1:N:788:ARG:HG3 | 1:N:814:SER:HB3 | 1.99 | 0.45 |
| 1:B:764:ASN:HA | 1:B:792:LYS:HD2 | 1.97 | 0.45 |
| 1:D:977:PHE:N | 1:D:1004:GLY:O | 2.47 | 0.45 |
| 1:N:343:ILE:O | 1:N:347:ILE:HG13 | 2.16 | 0.45 |
| 1:F:764:ASN:HA | 1:F:792:LYS:HD3 | 1.97 | 0.45 |
| 1:K:804:ILE:HG13 | 1:K:804:ILE:O | 2.17 | 0.45 |
| 1:H:145:ARG:NH1 | 1:H:615:ASP:OD1 | 2.49 | 0.45 |
| 1:F:969:PHE:CZ | 1:F:971:ASP:HB2 | 2.52 | 0.45 |
| 1:L:896:LEU:HD22 | 1:L:900:LEU:HD22 | 1.98 | 0.45 |
| 1:H:393:CYS:HB2 | 1:H:421:LEU:HD22 | 1.98 | 0.45 |
| 1:L:889:CYS:SG | 1:L:892:VAL:HG13 | 2.57 | 0.45 |
| 1:B:572:SER:HB2 | 1:B:604:ASN:HD21 | 1.81 | 0.45 |
| 1:B:855:ILE:HG13 | 1:B:887:PRO:HD3 | 1.99 | 0.45 |
| 1:P:360:THR:OG1 | 1:P:564:GLU:OE1 | 2.23 | 0.45 |
| 1:B:493:TYR:O | 1:B:497:SER:OG | 2.34 | 0.45 |
| 1:F:865:ASN:OD1 | 1:F:895:SER:OG | 2.34 | 0.45 |
| 1:B:499:THR:HA | 1:B:502:THR:HG23 | 1.98 | 0.45 |
| 1:P:115:LEU:HA | 1:P:130:LEU:HD22 | 1.98 | 0.45 |
| 1:D:591:ILE:O | 1:D:647:ARG:NH2 | 2.45 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:L:675:GLN:HG2 | 1:L:679:TYR:CE2 | 2.52 | 0.45 |
| 1:N:753:GLY:HA3 | 1:N:754:GLY:HA3 | 1.78 | 0.45 |
| 1:D:173:LYS:HA | 1:D:173:LYS:HD3 | 1.75 | 0.45 |
| 1:K:313:LEU:HA | 1:K:313:LEU:HD12 | 1.87 | 0.45 |
| 1:D:436:LYS:HE2 | 1:D:436:LYS:HB3 | 1.68 | 0.45 |
| 1:D:205:LEU:HD12 | 1:D:253:PHE:CG | 2.52 | 0.45 |
| 1:B:435:LEU:HD23 | 1:F:433:GLN:O | 2.16 | 0.45 |
| 1:L:440:LYS:HG2 | 1:L:441:PHE:O | 2.17 | 0.45 |
| 1:P:285:ARG:O | 1:P:520:GLY:HA3 | 2.17 | 0.45 |
| 1:K:140:TRP:O | 1:K:295:ALA:HA | 2.17 | 0.45 |
| 1:N:378:TYR:HD2 | 1:N:386:PHE:HD1 | 1.65 | 0.45 |
| 1:K:420:VAL:O | 1:K:424:ILE:HG13 | 2.17 | 0.45 |
| 1:N:974:THR:HG22 | 1:N:975:GLU:N | 2.30 | 0.45 |
| 1:H:345:CYS:O | 1:H:349:MET:HG3 | 2.16 | 0.45 |
| 1:B:418:GLU:HB2 | 1:B:439:TYR:CE2 | 2.52 | 0.45 |
| 1:F:1002:LEU:HD23 | 1:F:1007:PHE:HZ | 1.82 | 0.45 |
| 1:K:495:CYS:SG | 1:K:561:LEU:HD13 | 2.56 | 0.45 |
| 1:F:845:HIS:HA | 1:F:877:VAL:HG11 | 1.99 | 0.45 |
| 1:K:890:TRP:CZ2 | 1:F:580:GLN:HG2 | 2.52 | 0.45 |
| 1:N:142:LYS:HD2 | 1:N:168:GLU:OE2 | 2.16 | 0.45 |
| 1:P:393:CYS:HB2 | 1:P:421:LEU:CD2 | 2.47 | 0.45 |
| 1:L:338:PRO:O | 1:L:342:VAL:HG23 | 2.17 | 0.45 |
| 1:B:918:ARG:HB3 | 1:B:918:ARG:HE | 1.58 | 0.45 |
| 1:L:104:ASN:HB3 | 1:L:222:ASN:HB2 | 1.98 | 0.45 |
| 1:L:551:VAL:CG2 | 1:L:582:LYS:HG2 | 2.48 | 0.44 |
| 1:H:865:ASN:OD1 | 1:H:895:SER:OG | 2.35 | 0.44 |
| 1:H:665:THR:HB | 1:H:693:HIS:HB3 | 2.00 | 0.44 |
| 1:D:479:SER:HB2 | 1:D:516:GLY:HA3 | 1.98 | 0.44 |
| 1:H:498:SER:O | 1:H:502:THR:HG22 | 2.17 | 0.44 |
| 1:L:764:ASN:HA | 1:L:792:LYS:HD3 | 1.99 | 0.44 |
| 1:D:534:ILE:HG13 | 1:D:693:HIS:HB2 | 1.99 | 0.44 |
| 1:F:119:PRO:HB3 | 2:F:1101:ADP:O3' | 2.16 | 0.44 |
| 1:H:909:LEU:HD13 | 1:H:912:LEU:HB2 | 1.98 | 0.44 |
| 1:B:552:ASN:OD1 | 1:B:585:TYR:HB2 | 2.17 | 0.44 |
| 1:P:168:GLU:HA | 1:P:279:THR:O | 2.17 | 0.44 |
| 1:D:351:ARG:HE | 1:D:369:LEU:HD13 | 1.82 | 0.44 |
| 1:D:872:ILE:HA | 1:D:875:LEU:HG | 1.99 | 0.44 |
| 1:B:415:SER:O | 1:B:418:GLU:HG2 | 2.17 | 0.44 |
| 1:H:97:ASP:HA | 1:H:100:VAL:HG12 | 1.99 | 0.44 |
| 1:N:981:ALA:O | 1:N:984:VAL:HB | 2.16 | 0.44 |
| 1:N:832:LEU:HB2 | 1:N:858:ASN:CG | 2.38 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:896:LEU:HD22 | 1:B:900:LEU:HD22 | 2.00 | 0.44 |
| 1:N:691:ARG:HG2 | 1:N:715:HIS:HB3 | 1.98 | 0.44 |
| 1:L:756:ILE:H | 1:L:756:ILE:HG12 | 1.49 | 0.44 |
| 1:K:962:GLU:HA | 1:K:990:VAL:HG13 | 1.98 | 0.44 |
| 1:D:990:VAL:O | 1:D:994:LEU:HG | 2.18 | 0.44 |
| 1:K:920:ARG:NH2 | 1:K:922:GLU:OE2 | 2.50 | 0.44 |
| 1:F:979:PRO:O | 1:F:1010:TYR:OH | 2.27 | 0.44 |
| 1:D:420:VAL:O | 1:D:424:ILE:HG13 | 2.17 | 0.44 |
| 1:K:979:PRO:HB3 | 1:K:983:LEU:HD23 | 1.99 | 0.44 |
| 1:K:238:LYS:HE2 | 1:K:238:LYS:HB2 | 1.56 | 0.44 |
| 1:P:970:PHE:HE2 | 1:P:997:LEU:HD21 | 1.83 | 0.44 |
| 1:F:788:ARG:HH22 | 1:F:817:GLU:CD | 2.18 | 0.44 |
| 1:D:892:VAL:HG21 | 1:D:917:TRP:HA | 1.98 | 0.44 |
| 1:L:997:LEU:O | 1:L:1019:PHE:HB3 | 2.17 | 0.44 |
| 1:L:285:ARG:NH1 | 1:L:481:SER:OG | 2.50 | 0.44 |
| 1:L:335:MET:HE3 | 1:L:341:VAL:HA | 1.98 | 0.44 |
| 1:H:756:ILE:HG12 | 1:H:756:ILE:H | 1.45 | 0.44 |
| 1:N:683:ILE:O | 1:N:686:SER:OG | 2.26 | 0.44 |
| 1:B:969:PHE:HE1 | 1:B:971:ASP:HB2 | 1.81 | 0.44 |
| 1:K:931:LEU:HD22 | 1:K:964:LEU:HD21 | 1.99 | 0.44 |
| 1:B:823:GLN:HA | 1:B:850:LEU:HA | 2.00 | 0.44 |
| 1:H:746:LEU:HD12 | 1:H:746:LEU:HA | 1.87 | 0.44 |
| 1:N:832:LEU:HA | 1:N:832:LEU:HD23 | 1.89 | 0.44 |
| 1:D:914:LEU:HB3 | 1:D:917:TRP:CG | 2.52 | 0.44 |
| 1:N:325:ILE:HG12 | 1:N:331:LEU:HD23 | 2.00 | 0.44 |
| 1:F:825:MET:HB2 | 1:F:850:LEU:HD11 | 1.99 | 0.44 |
| 1:B:205:LEU:HB2 | 1:B:248:ASP:O | 2.17 | 0.44 |
| 1:F:267:GLU:OE1 | 1:F:270:ARG:NH1 | 2.40 | 0.44 |
| 1:F:918:ARG:HA | 1:F:946:GLY:O | 2.18 | 0.44 |
| 1:N:205:LEU:HB3 | 1:N:253:PHE:HB2 | 2.00 | 0.44 |
| 1:F:382:ALA:O | 1:F:384:GLY:N | 2.50 | 0.44 |
| 1:F:1017:GLY:C | 1:F:1019:PHE:H | 2.21 | 0.44 |
| 1:H:562:PHE:O | 1:H:565:SER:OG | 2.34 | 0.44 |
| 1:K:816:SER:O | 1:K:843:ASN:HB3 | 2.18 | 0.44 |
| 1:D:1002:LEU:HG | 1:D:1005:TRP:CE2 | 2.53 | 0.44 |
| 1:L:360:THR:OG1 | 1:L:564:GLU:OE1 | 2.27 | 0.44 |
| 1:H:646:PRO:O | 1:H:650:SER:OG | 2.36 | 0.44 |
| 1:H:925:LYS:O | 1:H:929:GLU:HG3 | 2.18 | 0.44 |
| 1:D:645:PRO:HA | 1:D:646:PRO:HD3 | 1.90 | 0.44 |
| 1:F:910:ALA:O | 1:F:940:GLN:N | 2.41 | 0.44 |
| 1:P:184:MET:HB2 | 1:P:184:MET:HE2 | 1.87 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:F:893:HIS:HB2 | 1:F:923:GLU:HG2 | 2.00 | 0.44 |
| 1:N:780:ALA:HB2 | 1:N:804:ILE:HB | 1.99 | 0.44 |
| 1:K:974:THR:HG23 | 1:K:975:GLU:O | 2.18 | 0.44 |
| 1:D:911:LYS:HG2 | 1:D:941:GLN:CG | 2.45 | 0.44 |
| 1:D:515:HIS:CE1 | 1:D:547:LYS:HD2 | 2.52 | 0.44 |
| 1:N:130:LEU:HD21 | 1:N:180:GLN:HB3 | 2.00 | 0.44 |
| 1:L:173:LYS:NZ | 1:L:337:THR:HG22 | 2.33 | 0.44 |
| 1:B:94:THR:OG1 | 1:B:97:ASP:HB2 | 2.18 | 0.44 |
| 1:P:588:SER:OG | 1:P:616:PHE:HA | 2.17 | 0.44 |
| 1:P:138:ILE:HG12 | 1:P:138:ILE:O | 2.16 | 0.44 |
| 1:D:335:MET:HG3 | 1:D:341:VAL:HG22 | 1.98 | 0.44 |
| 1:F:798:LEU:HD13 | 1:F:811:ILE:HD11 | 1.99 | 0.44 |
| 1:H:168:GLU:HA | 1:H:279:THR:O | 2.18 | 0.44 |
| 1:K:343:ILE:O | 1:K:347:ILE:HG13 | 2.18 | 0.44 |
| 1:L:743:ILE:HG12 | 1:L:770:LEU:HD12 | 2.00 | 0.44 |
| 1:P:474:LEU:HD21 | 1:P:505:VAL:HG22 | 2.00 | 0.44 |
| 1:D:583:SER:HB2 | 1:D:611:PHE:CE1 | 2.52 | 0.44 |
| 1:B:568:LYS:HD3 | 1:B:601:TYR:CZ | 2.52 | 0.44 |
| 1:N:799:THR:HG22 | 1:N:828:VAL:HG13 | 2.00 | 0.44 |
| 1:F:365:THR:O | 1:F:369:LEU:HB2 | 2.18 | 0.43 |
| 1:K:663:GLU:HG3 | 1:K:691:ARG:HB2 | 1.99 | 0.43 |
| 1:D:515:HIS:CD2 | 1:D:547:LYS:HD2 | 2.51 | 0.43 |
| 1:P:753:GLY:HA3 | 1:P:754:GLY:HA3 | 1.73 | 0.43 |
| 1:H:506:MET:HG3 | 1:H:575:PHE:CE1 | 2.53 | 0.43 |
| 1:P:827:LEU:N | 1:P:854:ASP:O | 2.46 | 0.43 |
| 1:N:198:ARG:N | 1:N:242:GLU:O | 2.49 | 0.43 |
| 1:L:1015:ILE:HG23 | 1:L:1016:LYS:H | 1.82 | 0.43 |
| 1:F:479:SER:O | 1:F:483:ILE:HG13 | 2.18 | 0.43 |
| 1:N:361:MET:O | 1:N:365:THR:OG1 | 2.30 | 0.43 |
| 1:N:360:THR:OG1 | 1:N:564:GLU:OE1 | 2.21 | 0.43 |
| 1:P:822:LEU:HD23 | 1:P:822:LEU:HA | 1.86 | 0.43 |
| 1:H:923:GLU:OE1 | 1:H:923:GLU:N | 2.51 | 0.43 |
| 1:P:975:GLU:C | 1:P:977:PHE:N | 2.71 | 0.43 |
| 1:K:747:HIS:NE2 | 1:K:772:ASP:OD1 | 2.42 | 0.43 |
| 1:N:941:GLN:HA | 1:N:967:LEU:CD1 | 2.47 | 0.43 |
| 1:F:393:CYS:HB2 | 1:F:421:LEU:CD2 | 2.48 | 0.43 |
| 1:N:240:HIS:HB3 | 1:N:241:LYS:H | 1.52 | 0.43 |
| 1:F:900:LEU:HD22 | 1:F:930:PHE:CD2 | 2.53 | 0.43 |
| 1:F:329:ARG:O | 1:F:333:ASN:ND2 | 2.51 | 0.43 |
| 1:K:392:TYR:OH | 1:K:418:GLU:OE2 | 2.27 | 0.43 |
| 1:B:463:GLU:HA | 1:B:464:PRO:HD2 | 1.80 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:313:LEU:HA | 1:H:313:LEU:HD12 | 1.83 | 0.43 |
| 1:N:393:CYS:HB2 | 1:N:421:LEU:CD2 | 2.49 | 0.43 |
| 1:L:787:LEU:HD13 | 1:L:815:LEU:HD21 | 2.00 | 0.43 |
| 1:F:346:ALA:HA | 1:F:349:MET:HE2 | 2.00 | 0.43 |
| 1:N:499:THR:O | 1:N:502:THR:HG23 | 2.18 | 0.43 |
| 1:H:910:ALA:O | 1:H:940:GLN:N | 2.41 | 0.43 |
| 1:L:599:PHE:CD1 | 1:L:651:LEU:HD22 | 2.52 | 0.43 |
| 1:L:145:ARG:CG | 1:L:523:VAL:CB | 2.95 | 0.43 |
| 1:K:715:HIS:ND1 | 1:K:716:THR:HG22 | 2.33 | 0.43 |
| 1:D:335:MET:HE3 | 1:D:341:VAL:HA | 1.99 | 0.43 |
| 1:K:833:THR:O | 1:K:836:SER:OG | 2.31 | 0.43 |
| 1:L:872:ILE:HA | 1:L:875:LEU:HG | 2.01 | 0.43 |
| 1:P:359:GLN:NE2 | 1:P:493:TYR:OH | 2.47 | 0.43 |
| 1:D:534:ILE:CG1 | 1:D:693:HIS:HB2 | 2.49 | 0.43 |
| 1:H:756:ILE:HG22 | 1:H:783:LEU:HD13 | 2.01 | 0.43 |
| 1:L:115:LEU:HA | 1:L:130:LEU:HD22 | 2.00 | 0.43 |
| 1:D:161:LEU:HD21 | 1:D:276:ILE:HD11 | 2.00 | 0.43 |
| 1:K:337:THR:HA | 1:K:338:PRO:HD3 | 1.79 | 0.43 |
| 1:N:138:ILE:O | 1:N:138:ILE:HG12 | 2.19 | 0.43 |
| 1:N:931:LEU:HD21 | 1:N:936:LEU:HB2 | 2.01 | 0.43 |
| 1:P:322:TRP:CE3 | 1:P:325:ILE:HD12 | 2.54 | 0.43 |
| 1:N:568:LYS:HB3 | 1:N:601:TYR:CD2 | 2.53 | 0.43 |
| 1:N:478:VAL:O | 1:N:512:VAL:HG13 | 2.18 | 0.43 |
| 1:B:436:LYS:HE3 | 1:F:217:TYR:CZ | 2.54 | 0.43 |
| 1:P:968:VAL:O | 1:P:998:GLN:N | 2.49 | 0.43 |
| 1:F:266:LYS:HA | 1:F:290:VAL:HG11 | 1.99 | 0.43 |
| 1:D:410:PRO:HG3 | 1:D:418:GLU:HG3 | 2.00 | 0.43 |
| 1:F:980:ASP:N | 1:F:980:ASP:OD2 | 2.51 | 0.43 |
| 1:B:712:LYS:HD2 | 1:B:712:LYS:C | 2.39 | 0.43 |
| 1:H:962:GLU:HA | 1:H:990:VAL:HG13 | 2.00 | 0.43 |
| 1:F:240:HIS:CG | 1:F:241:LYS:N | 2.86 | 0.43 |
| 1:L:371:ILE:HG13 | 1:L:372:GLN:N | 2.33 | 0.43 |
| 1:N:962:GLU:HA | 1:N:994:LEU:HD21 | 1.99 | 0.43 |
| 1:B:245:PHE:HB2 | 1:B:275:VAL:HG12 | 2.00 | 0.43 |
| 1:D:817:GLU:HB3 | 1:D:818:GLU:HG3 | 2.00 | 0.43 |
| 1:N:934:ASN:HB3 | 1:N:935:PRO:O | 2.18 | 0.43 |
| 1:F:285:ARG:O | 1:F:520:GLY:HA3 | 2.19 | 0.43 |
| 1:H:145:ARG:HH21 | 1:H:667:ARG:HH21 | 1.65 | 0.43 |
| 1:B:890:TRP:CZ3 | 1:B:918:ARG:HD3 | 2.54 | 0.43 |
| 1:B:401:VAL:HG11 | 1:B:490:LEU:HD22 | 2.00 | 0.43 |
| 1:L:823:GLN:HA | 1:L:850:LEU:HA | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:N:96:GLU:H | 1:N:96:GLU:CD | 2.21 | 0.43 |
| 1:B:416:MET:H | 1:B:416:MET:HG2 | 1.38 | 0.43 |
| 1:L:920:ARG:HA | 1:L:948:CYS:O | 2.19 | 0.43 |
| 1:D:285:ARG:O | 1:D:520:GLY:HA3 | 2.18 | 0.43 |
| 1:B:267:GLU:HB3 | 1:B:269:HIS:CE1 | 2.53 | 0.43 |
| 1:F:205:LEU:HB2 | 1:F:248:ASP:O | 2.19 | 0.43 |
| 1:H:347:ILE:HA | 1:H:369:LEU:HD21 | 2.01 | 0.43 |
| 1:D:573:GLN:NE2 | 1:F:862:LYS:HB3 | 2.34 | 0.43 |
| 1:N:855:ILE:HG13 | 1:N:887:PRO:HD3 | 2.01 | 0.43 |
| 1:N:947:HIS:O | 1:N:947:HIS:CG | 2.71 | 0.43 |
| 1:L:522:SER:C | 1:L:523:VAL:O | 2.55 | 0.43 |
| 1:N:981:ALA:HA | 1:N:984:VAL:HB | 2.01 | 0.43 |
| 1:L:538:ARG:HE | 1:L:538:ARG:HB3 | 1.51 | 0.43 |
| 1:L:1017:GLY:C | 1:L:1019:PHE:H | 2.22 | 0.43 |
| 1:B:551:VAL:CG1 | 1:B:582:LYS:HG2 | 2.49 | 0.43 |
| 1:P:142:LYS:HD2 | 1:P:168:GLU:OE2 | 2.19 | 0.43 |
| 1:N:502:THR:HG21 | 1:N:565:SER:HB2 | 2.01 | 0.43 |
| 1:K:449:TYR:OH | 1:K:453:ARG:NH1 | 2.41 | 0.43 |
| 1:L:345:CYS:O | 1:L:349:MET:HG3 | 2.19 | 0.43 |
| 1:B:743:ILE:HG13 | 1:B:773:ILE:HD11 | 1.99 | 0.43 |
| 1:F:1001:LYS:HG3 | 1:F:1022:VAL:HB | 2.01 | 0.43 |
| 1:L:922:GLU:HG2 | 1:L:922:GLU:H | 1.28 | 0.42 |
| 1:N:931:LEU:HD11 | 1:N:964:LEU:HD21 | 2.01 | 0.42 |
| 1:B:859:TYR:CE1 | 1:B:889:CYS:HA | 2.53 | 0.42 |
| 1:K:308:LEU:HD13 | 2:K:1101:ADP:C2 | 2.54 | 0.42 |
| 1:F:409:GLU:HB2 | 1:F:436:LYS:HD3 | 1.99 | 0.42 |
| 1:K:816:SER:HB2 | 1:K:843:ASN:HB2 | 2.00 | 0.42 |
| 1:K:746:LEU:HD12 | 1:K:746:LEU:HA | 1.75 | 0.42 |
| 1:L:746:LEU:HA | 1:L:746:LEU:HD12 | 1.92 | 0.42 |
| 1:F:205:LEU:HB3 | 1:F:253:PHE:HB2 | 2.01 | 0.42 |
| 1:H:679:TYR:O | 1:H:683:ILE:HG13 | 2.19 | 0.42 |
| 1:N:143:ASP:O | 1:N:144:HIS:CG | 2.72 | 0.42 |
| 1:B:811:ILE:O | 1:B:815:LEU:HG | 2.19 | 0.42 |
| 1:H:827:LEU:HD13 | 1:H:827:LEU:HA | 1.84 | 0.42 |
| 1:H:588:SER:OG | 1:H:615:ASP:O | 2.31 | 0.42 |
| 1:H:771:ASP:OD1 | 1:H:800:HIS:HB2 | 2.19 | 0.42 |
| 1:F:1012:ILE:O | 1:F:1015:ILE:HG22 | 2.19 | 0.42 |
| 1:F:919:LEU:HD22 | 1:F:923:GLU:HB3 | 2.02 | 0.42 |
| 1:L:309:ILE:HD11 | 1:L:335:MET:HE2 | 2.00 | 0.42 |
| 1:F:1001:LYS:HA | 1:F:1022:VAL:HB | 2.01 | 0.42 |
| 1:N:143:ASP:HB3 | 1:N:149:VAL:CG2 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:920:ARG:HB2 | 1:P:922:GLU:HG2 | 2.00 | 0.42 |
| 1:K:562:PHE:HB2 | 1:K:575:PHE:CE1 | 2.54 | 0.42 |
| 1:N:645:PRO:HA | 1:N:646:PRO:HD3 | 1.91 | 0.42 |
| 1:D:974:THR:HG23 | 1:D:975:GLU:N | 2.33 | 0.42 |
| 1:D:168:GLU:HA | 1:D:279:THR:O | 2.18 | 0.42 |
| 1:N:791:LYS:HB3 | 1:N:791:LYS:HE3 | 1.86 | 0.42 |
| 1:H:832:LEU:HD23 | 1:H:832:LEU:HA | 1.87 | 0.42 |
| 1:P:911:LYS:HG2 | 1:P:941:GLN:HG2 | 2.01 | 0.42 |
| 1:H:765:LEU:HD21 | 1:H:768:LEU:HD13 | 2.00 | 0.42 |
| 1:H:986:LYS:O | 1:H:990:VAL:HG23 | 2.18 | 0.42 |
| 1:D:362:LEU:HA | 1:D:362:LEU:HD12 | 1.89 | 0.42 |
| 1:L:816:SER:HB2 | 1:L:843:ASN:CB | 2.48 | 0.42 |
| 1:H:218:ASP:HA | 1:L:435:LEU:HD21 | 2.01 | 0.42 |
| 1:H:124:ILE:HD11 | 1:H:370:LEU:HD11 | 2.02 | 0.42 |
| 1:N:507:ARG:HG2 | 1:P:890:TRP:CE3 | 2.53 | 0.42 |
| 1:P:865:ASN:OD1 | 1:P:895:SER:OG | 2.36 | 0.42 |
| 1:P:895:SER:O | 1:P:899:LEU:N | 2.42 | 0.42 |
| 1:K:480:ILE:HG23 | 1:K:514:GLN:O | 2.20 | 0.42 |
| 1:B:986:LYS:NZ | 1:F:963:ASN:OD1 | 2.42 | 0.42 |
| 1:H:911:LYS:HG2 | 1:H:941:GLN:HG2 | 2.01 | 0.42 |
| 1:N:313:LEU:HD12 | 1:N:313:LEU:HA | 1.88 | 0.42 |
| 1:L:593:ASP:OD2 | 1:L:647:ARG:NH2 | 2.40 | 0.42 |
| 1:K:803:ASP:OD2 | 1:F:462:LYS:HG2 | 2.19 | 0.42 |
| 1:F:126:ILE:HG23 | 1:F:312:VAL:HG11 | 2.02 | 0.42 |
| 1:L:669:ILE:HB | 1:L:697:CYS:SG | 2.60 | 0.42 |
| 1:K:572:SER:HG | 1:K:604:ASN:HD21 | 1.57 | 0.42 |
| 1:K:518:LEU:HD11 | 1:K:547:LYS:HG2 | 2.01 | 0.42 |
| 1:L:910:ALA:O | 1:L:940:GLN:N | 2.45 | 0.42 |
| 1:L:936:LEU:HB3 | 1:L:939:LEU:HB2 | 2.00 | 0.42 |
| 1:H:541:THR:HG23 | 1:H:544:ASP:H | 1.83 | 0.42 |
| 1:K:498:SER:O | 1:K:502:THR:HG23 | 2.19 | 0.42 |
| 1:P:595:LEU:HD13 | 1:P:595:LEU:HA | 1.79 | 0.42 |
| 1:L:205:LEU:HD12 | 1:L:205:LEU:HA | 1.88 | 0.42 |
| 1:H:393:CYS:HB2 | 1:H:421:LEU:CD2 | 2.49 | 0.42 |
| 1:L:990:VAL:O | 1:L:994:LEU:HG | 2.20 | 0.42 |
| 1:N:537:LEU:HD21 | 1:N:740:ASN:HB3 | 2.01 | 0.42 |
| 1:K:252:GLU:HA | 1:K:406:PHE:CE2 | 2.54 | 0.42 |
| 1:P:189:GLY:N | 1:P:190:GLY:HA3 | 2.33 | 0.42 |
| 1:H:238:LYS:O | 1:H:240:HIS:ND1 | 2.49 | 0.42 |
| 1:H:915:LYS:HG2 | 1:H:945:ALA:HB3 | 2.01 | 0.42 |
| 1:D:822:LEU:HD23 | 1:D:822:LEU:HA | 1.91 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:832:LEU:HD23 | 1:P:832:LEU:HA | 1.85 | 0.42 |
| 1:P:543:GLN:O | 1:P:547:LYS:HG3 | 2.19 | 0.42 |
| 1:K:93:VAL:HG22 | 1:K:231:THR:HG22 | 2.00 | 0.42 |
| 1:B:969:PHE:C | 1:B:969:PHE:CD1 | 2.93 | 0.42 |
| 1:D:170:GLU:O | 1:D:175:LYS:NZ | 2.53 | 0.42 |
| 1:K:479:SER:O | 1:K:483:ILE:HG13 | 2.20 | 0.42 |
| 1:N:775:MET:SD | 1:N:801:LEU:HD22 | 2.60 | 0.42 |
| 1:B:562:PHE:HB2 | 1:B:575:PHE:CE1 | 2.53 | 0.42 |
| 1:B:265:ILE:HG23 | 1:B:277:VAL:HG21 | 2.02 | 0.42 |
| 1:D:313:LEU:HA | 1:D:313:LEU:HD12 | 1.86 | 0.42 |
| 1:P:955:LEU:CD1 | 1:P:983:LEU:N | 2.82 | 0.42 |
| 1:L:874:ARG:CG | 1:L:874:ARG:HH11 | 2.26 | 0.42 |
| 1:D:341:VAL:O | 1:D:344:THR:OG1 | 2.35 | 0.42 |
| 1:B:524:THR:O | 1:B:527:PRO:HD2 | 2.19 | 0.42 |
| 1:N:429:LYS:O | 1:N:431:THR:HG23 | 2.20 | 0.42 |
| 1:N:931:LEU:CD2 | 1:N:936:LEU:HB2 | 2.50 | 0.42 |
| 1:N:852:ILE:HD13 | 1:N:883:THR:HB | 2.02 | 0.42 |
| 1:H:333:ASN:HA | 1:H:336:LYS:NZ | 2.34 | 0.42 |
| 1:B:675:GLN:HG2 | 1:B:679:TYR:CE2 | 2.54 | 0.42 |
| 1:B:130:LEU:O | 1:B:181:ARG:NH2 | 2.52 | 0.42 |
| 1:K:474:LEU:HD23 | 1:K:477:MET:HE1 | 2.01 | 0.42 |
| 1:F:914:LEU:HB3 | 1:F:917:TRP:CG | 2.55 | 0.42 |
| 1:B:285:ARG:NH1 | 1:B:521:LEU:HD21 | 2.34 | 0.42 |
| 1:K:599:PHE:O | 1:K:657:GLN:NE2 | 2.52 | 0.42 |
| 1:K:664:VAL:HG22 | 1:K:692:LEU:HD23 | 2.01 | 0.42 |
| 1:K:145:ARG:NH1 | 1:K:615:ASP:OD2 | 2.52 | 0.42 |
| 1:H:991:LEU:HD13 | 1:H:997:LEU:CD2 | 2.50 | 0.42 |
| 1:F:405:LYS:HE2 | 1:F:405:LYS:HB3 | 1.82 | 0.42 |
| 1:H:96:GLU:O | 1:H:100:VAL:HG12 | 2.19 | 0.42 |
| 1:N:990:VAL:O | 1:N:994:LEU:HG | 2.20 | 0.42 |
| 1:L:854:ASP:OD2 | 1:L:856:SER:OG | 2.34 | 0.42 |
| 1:N:964:LEU:HG | 1:N:964:LEU:H | 1.48 | 0.42 |
| 1:N:269:HIS:CD2 | 1:N:269:HIS:H | 2.37 | 0.42 |
| 1:P:460:THR:HG21 | 1:P:498:SER:OG | 2.20 | 0.42 |
| 1:N:605:CYS:O | 1:N:609:LEU:HG | 2.20 | 0.42 |
| 1:D:764:ASN:HA | 1:D:792:LYS:HD3 | 2.01 | 0.42 |
| 1:L:825:MET:HG2 | 1:L:827:LEU:HD13 | 2.02 | 0.42 |
| 1:K:345:CYS:O | 1:K:349:MET:HG3 | 2.19 | 0.42 |
| 1:P:480:ILE:HG13 | 1:P:514:GLN:O | 2.20 | 0.42 |
| 1:K:777:GLU:O | 1:K:781:LYS:HG3 | 2.20 | 0.42 |
| 1:D:677:ILE:HG23 | 1:D:707:VAL:HG22 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:282:GLU:H | 1:K:282:GLU:HG3 | 1.65 | 0.42 |
| 1:P:712:LYS:HD2 | 1:P:712:LYS:HA | 1.93 | 0.42 |
| 1:L:333:ASN:HA | 1:L:336:LYS:HZ3 | 1.85 | 0.42 |
| 1:K:288:ARG:NH2 | 1:K:522:SER:O | 2.47 | 0.42 |
| 1:D:325:ILE:HD13 | 1:D:335:MET:HG2 | 2.01 | 0.42 |
| 1:L:970:PHE:HZ | 1:L:991:LEU:HD11 | 1.84 | 0.42 |
| 1:H:582:LYS:O | 1:H:610:ASP:N | 2.52 | 0.42 |
| 1:K:248:ASP:HA | 1:K:278:THR:HB | 2.01 | 0.42 |
| 1:L:653:PHE:O | 1:L:654:ASN:HB2 | 2.20 | 0.42 |
| 1:K:571:LEU:HB3 | 1:K:575:PHE:HD2 | 1.85 | 0.42 |
| 1:B:945:ALA:O | 1:B:946:GLY:C | 2.58 | 0.42 |
| 1:D:859:TYR:HH | 1:D:890:TRP:HD1 | 1.66 | 0.42 |
| 1:D:429:LYS:HB2 | 1:D:439:TYR:CD2 | 2.55 | 0.42 |
| 1:B:478:VAL:O | 1:B:512:VAL:HG13 | 2.20 | 0.42 |
| 1:H:931:LEU:HA | 1:H:931:LEU:HD23 | 1.81 | 0.42 |
| 1:B:1018:THR:OG1 | 1:B:1018:THR:O | 2.37 | 0.42 |
| 1:K:537:LEU:HD21 | 1:K:740:ASN:HB3 | 2.01 | 0.41 |
| 1:F:549:ILE:O | 1:F:552:ASN:HB2 | 2.19 | 0.41 |
| 1:P:324:GLN:OE1 | 1:P:353:GLU:HG2 | 2.20 | 0.41 |
| 1:N:591:ILE:HB | 1:N:647:ARG:HG2 | 2.02 | 0.41 |
| 1:K:813:LYS:HE3 | 1:K:817:GLU:HG3 | 2.01 | 0.41 |
| 1:B:854:ASP:HA | 1:B:885:MET:HB2 | 2.02 | 0.41 |
| 1:L:518:LEU:HA | 1:L:521:LEU:HD22 | 2.02 | 0.41 |
| 1:P:756:ILE:HG22 | 1:P:783:LEU:HD13 | 2.02 | 0.41 |
| 1:N:740:ASN:ND2 | 1:N:767:ARG:HB2 | 2.35 | 0.41 |
| 1:K:743:ILE:HG13 | 1:K:743:ILE:O | 2.20 | 0.41 |
| 1:B:986:LYS:O | 1:B:990:VAL:HG23 | 2.20 | 0.41 |
| 1:D:925:LYS:O | 1:D:929:GLU:HG3 | 2.19 | 0.41 |
| 1:P:869:GLN:NE2 | 1:P:898:LYS:HD3 | 2.34 | 0.41 |
| 1:K:507:ARG:NH1 | 1:K:574:GLU:HG3 | 2.34 | 0.41 |
| 1:N:770:LEU:HD12 | 1:N:770:LEU:HA | 1.93 | 0.41 |
| 1:B:282:GLU:H | 1:B:282:GLU:HG3 | 1.63 | 0.41 |
| 1:N:588:SER:HA | 1:N:591:ILE:HD11 | 2.03 | 0.41 |
| 1:F:361:MET:O | 1:F:365:THR:OG1 | 2.29 | 0.41 |
| 1:N:480:ILE:HG23 | 1:N:514:GLN:O | 2.20 | 0.41 |
| 1:N:339:LEU:O | 1:N:343:ILE:HG13 | 2.20 | 0.41 |
| 1:F:900:LEU:HD22 | 1:F:930:PHE:CG | 2.55 | 0.41 |
| 1:L:817:GLU:HB3 | 1:L:818:GLU:HG3 | 2.02 | 0.41 |
| 1:D:229:LYS:HB3 | 1:D:230:PRO:HD3 | 2.02 | 0.41 |
| 1:P:970:PHE:HZ | 1:P:991:LEU:HD21 | 1.84 | 0.41 |
| 1:B:225:ASP:HB3 | 1:F:409:GLU:O | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:568:LYS:HD3 | 1:H:601:TYR:CE1 | 2.56 | 0.41 |
| 1:F:824:GLU:HG2 | 1:F:852:ILE:HB | 2.02 | 0.41 |
| 1:H:492:LEU:HG | 1:H:564:GLU:HG3 | 2.03 | 0.41 |
| 1:F:345:CYS:O | 1:F:349:MET:HG3 | 2.20 | 0.41 |
| 1:F:205:LEU:HD12 | 1:F:205:LEU:HA | 1.89 | 0.41 |
| 1:N:619:ARG:HH11 | 1:N:645:PRO:HB3 | 1.86 | 0.41 |
| 1:H:230:PRO:HG3 | 1:L:256:GLN:HG2 | 2.02 | 0.41 |
| 1:P:776:ASN:H | 1:P:779:ASP:HB2 | 1.85 | 0.41 |
| 1:N:158:LEU:O | 1:N:161:LEU:HG | 2.20 | 0.41 |
| 1:L:752:PRO:HA | 1:L:757:ASP:OD1 | 2.20 | 0.41 |
| 1:N:906:THR:O | 1:N:909:LEU:HB2 | 2.20 | 0.41 |
| 1:H:167:ILE:HB | 1:H:278:THR:HG22 | 2.01 | 0.41 |
| 1:N:479:SER:O | 1:N:483:ILE:HG13 | 2.21 | 0.41 |
| 1:B:920:ARG:HA | 1:B:948:CYS:O | 2.20 | 0.41 |
| 1:K:173:LYS:HD3 | 1:K:173:LYS:HA | 1.68 | 0.41 |
| 1:N:334:LEU:HA | 1:N:334:LEU:HD13 | 1.88 | 0.41 |
| 1:D:891:ASP:N | 1:D:891:ASP:OD1 | 2.44 | 0.41 |
| 1:K:322:TRP:CE3 | 1:K:325:ILE:HD12 | 2.55 | 0.41 |
| 1:F:716:THR:HG22 | 1:F:740:ASN:HD22 | 1.85 | 0.41 |
| 1:L:168:GLU:HB3 | 1:L:284:LEU:HD13 | 2.01 | 0.41 |
| 1:P:416:MET:O | 1:P:420:VAL:HG23 | 2.20 | 0.41 |
| 1:F:164:PRO:HG2 | 1:F:290:VAL:HG12 | 2.02 | 0.41 |
| 1:D:418:GLU:H | 1:D:418:GLU:HG2 | 1.59 | 0.41 |
| 1:B:740:ASN:HD22 | 1:B:767:ARG:HB2 | 1.86 | 0.41 |
| 1:D:797:HIS:CE1 | 1:D:826:LYS:HG3 | 2.56 | 0.41 |
| 1:L:351:ARG:HE | 1:L:369:LEU:HG | 1.84 | 0.41 |
| 1:N:434:ARG:NH2 | 1:N:438:THR:HG21 | 2.34 | 0.41 |
| 1:P:799:THR:HA | 1:P:828:VAL:O | 2.20 | 0.41 |
| 1:N:694:ILE:HD12 | 1:N:719:VAL:HG22 | 2.03 | 0.41 |
| 1:N:371:ILE:O | 1:N:375:SER:HB3 | 2.21 | 0.41 |
| 1:D:398:LEU:HD23 | 1:D:398:LEU:HA | 1.91 | 0.41 |
| 1:F:1018:THR:OG1 | 1:F:1018:THR:O | 2.39 | 0.41 |
| 1:K:361:MET:O | 1:K:365:THR:OG1 | 2.31 | 0.41 |
| 1:B:595:LEU:HA | 1:B:595:LEU:HD13 | 1.76 | 0.41 |
| 1:K:228:SER:OG | 1:K:231:THR:OG1 | 2.17 | 0.41 |
| 1:F:888:TRP:HA | 1:F:892:VAL:HG11 | 2.02 | 0.41 |
| 1:D:252:GLU:HA | 1:D:406:PHE:CE2 | 2.55 | 0.41 |
| 1:H:750:GLN:HG3 | 1:H:756:ILE:HD11 | 2.03 | 0.41 |
| 1:B:434:ARG:HB3 | 1:B:436:LYS:O | 2.20 | 0.41 |
| 1:H:306:LYS:HD2 | 1:H:322:TRP:CE2 | 2.56 | 0.41 |
| 1:F:653:PHE:HA | 1:F:656:LYS:HD2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:855:ILE:O | 1:P:858:ASN:ND2 | 2.53 | 0.41 |
| 1:N:968:VAL:O | 1:N:998:GLN:N | 2.44 | 0.41 |
| 1:K:669:ILE:HB | 1:K:697:CYS:SG | 2.61 | 0.41 |
| 1:B:832:LEU:HB2 | 1:B:858:ASN:OD1 | 2.20 | 0.41 |
| 1:F:347:ILE:O | 1:F:351:ARG:N | 2.52 | 0.41 |
| 1:K:890:TRP:CH2 | 1:F:580:GLN:HG2 | 2.55 | 0.41 |
| 1:K:920:ARG:HE | 1:K:920:ARG:HB2 | 1.73 | 0.41 |
| 1:F:617:TYR:C | 1:F:619:ARG:H | 2.23 | 0.41 |
| 1:F:800:HIS:H | 1:F:829:ALA:HB3 | 1.86 | 0.41 |
| 1:P:872:ILE:HA | 1:P:875:LEU:HG | 2.02 | 0.41 |
| 1:N:266:LYS:HA | 1:N:290:VAL:HG21 | 2.02 | 0.41 |
| 1:P:924:ILE:HD13 | 1:P:924:ILE:HA | 1.70 | 0.41 |
| 1:D:920:ARG:HA | 1:D:920:ARG:HD2 | 1.85 | 0.41 |
| 1:B:221:LEU:HD12 | 1:B:221:LEU:HA | 1.96 | 0.41 |
| 1:F:931:LEU:HA | 1:F:931:LEU:HD23 | 1.83 | 0.41 |
| 1:N:274:MET:HE3 | 1:N:274:MET:HB3 | 1.73 | 0.41 |
| 1:B:672:LEU:HD12 | 1:B:676:ASP:HB3 | 2.02 | 0.41 |
| 1:B:672:LEU:HB2 | 1:B:699:ALA:HB1 | 2.02 | 0.41 |
| 1:D:321:LEU:O | 1:D:325:ILE:HG13 | 2.21 | 0.41 |
| 1:B:936:LEU:HD12 | 1:B:936:LEU:HA | 1.78 | 0.41 |
| 1:F:421:LEU:HB2 | 1:F:427:LEU:HD12 | 2.02 | 0.41 |
| 1:B:679:TYR:O | 1:B:683:ILE:HG13 | 2.21 | 0.41 |
| 1:N:719:VAL:HG11 | 1:N:724:LEU:HD13 | 2.02 | 0.41 |
| 1:N:744:HIS:NE2 | 1:N:771:ASP:OD2 | 2.54 | 0.41 |
| 1:N:337:THR:HA | 1:N:338:PRO:HD3 | 1.89 | 0.41 |
| 1:L:800:HIS:H | 1:L:829:ALA:HB3 | 1.86 | 0.41 |
| 1:D:745:ARG:HA | 1:D:772:ASP:HB3 | 2.03 | 0.41 |
| 1:K:206:ARG:HG2 | 1:K:207:SER:N | 2.35 | 0.41 |
| 1:L:576:GLU:HB2 | 1:L:604:ASN:HD22 | 1.85 | 0.41 |
| 1:P:987:LEU:O | 1:P:991:LEU:HB2 | 2.21 | 0.41 |
| 1:K:531:GLN:NE2 | 1:K:744:HIS:HE1 | 2.18 | 0.41 |
| 1:D:568:LYS:HB3 | 1:D:601:TYR:CD2 | 2.56 | 0.41 |
| 1:B:420:VAL:O | 1:B:423:THR:OG1 | 2.26 | 0.41 |
| 1:N:621:THR:HG21 | 1:N:679:TYR:HB2 | 2.03 | 0.41 |
| 1:B:376:HIS:HE2 | 1:H:107:ASP:CG | 2.25 | 0.41 |
| 1:B:813:LYS:O | 1:B:817:GLU:N | 2.53 | 0.41 |
| 1:P:680:LEU:HB3 | 1:P:684:PHE:CE2 | 2.55 | 0.41 |
| 1:K:918:ARG:NH2 | 1:K:975:GLU:OE1 | 2.53 | 0.41 |
| 1:B:712:LYS:O | 1:B:712:LYS:HD2 | 2.20 | 0.41 |
| 1:B:990:VAL:O | 1:B:994:LEU:HG | 2.20 | 0.41 |
| 1:P:97:ASP:HA | 1:P:100:VAL:HG22 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:477:MET:HE1 | 1:L:491:LEU:HD21 | 2.02 | 0.41 |
| 1:F:832:LEU:HB2 | 1:F:858:ASN:CG | 2.42 | 0.41 |
| 1:N:189:GLY:HA3 | 1:N:190:GLY:HA2 | 1.56 | 0.41 |
| 1:F:173:LYS:HA | 1:F:173:LYS:HD3 | 1.77 | 0.41 |
| 1:D:303:ASP:OD2 | 1:D:303:ASP:N | 2.54 | 0.41 |
| 1:L:324:GLN:HE22 | 1:L:354:PHE:H | 1.67 | 0.41 |
| 1:P:338:PRO:O | 1:P:342:VAL:HG23 | 2.21 | 0.41 |
| 1:B:645:PRO:HA | 1:B:646:PRO:HD3 | 1.95 | 0.41 |
| 1:B:555:VAL:O | 1:B:559:ILE:HG13 | 2.21 | 0.41 |
| 1:B:746:LEU:HD23 | 1:B:746:LEU:HA | 1.65 | 0.41 |
| 1:B:383:SER:HB3 | 1:B:384:GLY:H | 1.57 | 0.41 |
| 1:H:813:LYS:HD3 | 1:H:817:GLU:OE2 | 2.21 | 0.41 |
| 1:K:914:LEU:HB3 | 1:K:917:TRP:CD1 | 2.56 | 0.41 |
| 1:K:925:LYS:HA | 1:K:956:TYR:HE2 | 1.86 | 0.41 |
| 1:F:859:TYR:CE1 | 1:F:889:CYS:HA | 2.56 | 0.41 |
| 1:B:918:ARG:HG2 | 1:B:918:ARG:H | 1.52 | 0.41 |
| 1:K:823:GLN:HA | 1:K:850:LEU:HA | 2.02 | 0.41 |
| 1:F:816:SER:HB2 | 1:F:843:ASN:CB | 2.52 | 0.40 |
| 1:B:614:LEU:HD23 | 1:B:616:PHE:CE2 | 2.56 | 0.40 |
| 1:D:665:THR:HG23 | 1:D:693:HIS:HB3 | 2.03 | 0.40 |
| 1:B:131:GLU:HA | 1:B:181:ARG:HH22 | 1.86 | 0.40 |
| 1:D:360:THR:OG1 | 1:D:564:GLU:OE1 | 2.25 | 0.40 |
| 1:P:612:VAL:O | 1:P:662:LEU:HD23 | 2.21 | 0.40 |
| 1:N:904:GLU:HG2 | 1:N:930:PHE:HE1 | 1.86 | 0.40 |
| 1:F:822:LEU:HD23 | 1:F:822:LEU:HA | 1.86 | 0.40 |
| 1:F:968:VAL:HG12 | 1:F:998:GLN:HB2 | 2.02 | 0.40 |
| 1:F:378:TYR:HD2 | 1:F:386:PHE:CD1 | 2.34 | 0.40 |
| 1:K:266:LYS:HA | 1:K:290:VAL:HG21 | 2.03 | 0.40 |
| 1:H:343:ILE:O | 1:H:347:ILE:HG13 | 2.20 | 0.40 |
| 1:K:562:PHE:O | 1:K:565:SER:OG | 2.32 | 0.40 |
| 1:P:751:LEU:HD23 | 1:P:752:PRO:O | 2.22 | 0.40 |
| 1:H:799:THR:HA | 1:H:828:VAL:O | 2.20 | 0.40 |
| 1:N:506:MET:HG3 | 1:N:575:PHE:CE1 | 2.56 | 0.40 |
| 1:D:205:LEU:CD2 | 1:D:247:LEU:HB3 | 2.45 | 0.40 |
| 1:N:98:LEU:HD13 | 1:N:235:LEU:HD21 | 2.02 | 0.40 |
| 1:H:816:SER:HB2 | 1:H:843:ASN:CB | 2.51 | 0.40 |
| 1:P:882:THR:O | 1:P:910:ALA:N | 2.51 | 0.40 |
| 1:L:92:GLN:O | 1:L:93:VAL:HG22 | 2.22 | 0.40 |
| 1:K:161:LEU:HD21 | 1:K:276:ILE:HD11 | 2.03 | 0.40 |
| 1:B:240:HIS:HB3 | 1:B:241:LYS:H | 1.50 | 0.40 |
| 1:D:400:GLY:O | 1:D:404:HIS:N | 2.55 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:399:GLU:OE1 | 1:L:473:TYR:OH | 2.29 | 0.40 |
| 1:H:134:PHE:CZ | 1:H:181:ARG:HG2 | 2.56 | 0.40 |
| 1:N:925:LYS:O | 1:N:929:GLU:HG2 | 2.21 | 0.40 |
| 1:F:239:LEU:HA | 1:F:239:LEU:HD22 | 1.89 | 0.40 |
| 1:L:656:LYS:HG2 | 1:L:656:LYS:H | 1.47 | 0.40 |
| 1:B:164:PRO:HG2 | 1:B:290:VAL:CG1 | 2.52 | 0.40 |
| 1:F:876:GLY:N | 1:F:902:GLN:HE21 | 2.19 | 0.40 |
| 1:H:503:ARG:HG3 | 1:H:571:LEU:CD1 | 2.51 | 0.40 |
| 1:H:495:CYS:HB3 | 1:H:502:THR:HB | 2.02 | 0.40 |
| 1:K:614:LEU:O | 1:K:664:VAL:HA | 2.21 | 0.40 |
| 1:H:216:LEU:HD11 | 1:H:245:PHE:HE1 | 1.86 | 0.40 |
| 1:F:915:LYS:HA | 1:F:945:ALA:HB3 | 2.03 | 0.40 |
| 1:D:931:LEU:HD23 | 1:D:931:LEU:HA | 1.82 | 0.40 |
| 1:N:769:ILE:HA | 1:N:797:HIS:HB2 | 2.03 | 0.40 |
| 1:N:223:ILE:HA | 1:N:224:PRO:HD3 | 1.91 | 0.40 |
| 1:B:344:THR:HB | 1:B:362:LEU:HD11 | 2.04 | 0.40 |
| 1:F:753:GLY:HA3 | 1:F:754:GLY:HA3 | 1.73 | 0.40 |
| 1:H:93:VAL:HG11 | 1:H:235:LEU:HD22 | 2.03 | 0.40 |
| 1:F:921:ASP:O | 1:F:925:LYS:HB2 | 2.21 | 0.40 |
| 1:N:543:GLN:O | 1:N:547:LYS:HG3 | 2.21 | 0.40 |
| 1:D:426:LEU:HA | 1:D:426:LEU:HD13 | 1.82 | 0.40 |
| 1:K:416:MET:O | 1:K:420:VAL:HG23 | 2.22 | 0.40 |
| 1:K:781:LYS:O | 1:K:785:GLU:HG3 | 2.21 | 0.40 |
| 1:N:909:LEU:O | 1:N:939:LEU:HA | 2.21 | 0.40 |
| 1:P:126:ILE:HG21 | 1:P:342:VAL:HG13 | 2.02 | 0.40 |
| 1:B:746:LEU:O | 1:B:747:HIS:HB2 | 2.22 | 0.40 |
| 1:N:126:ILE:HG21 | 1:N:342:VAL:HG13 | 2.03 | 0.40 |
| 1:D:813:LYS:HD2 | 1:D:839:VAL:HG11 | 2.04 | 0.40 |
| 1:B:724:LEU:HG | 1:B:728:ASP:HB2 | 2.04 | 0.40 |
| 1:P:568:LYS:HE2 | 1:P:568:LYS:HB2 | 1.95 | 0.40 |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:K:433:GLN:CD | 1:K:433:GLN:NE2[8_555] | 1.34 | 0.86 |
| 1:K:433:GLN:OE1 | 1:K:433:GLN:NE2[8_555] | 1.76 | 0.44 |

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 | B | 896/1024 (88%) | 875 (98%) | 21 (2%) | 0 | 100 | 100 |
| 1 | D | 893/1024 (87%) | 864 (97%) | 28 (3%) | 1 (0%) | 56 | 91 |
| 1 | F | 892/1024 (87%) | 868 (97%) | 23 (3%) | 1 (0%) | 56 | 91 |
| 1 | H | 887/1024 (87%) | 862 (97%) | 25 (3%) | 0 | 100 | 100 |
| 1 | K | 895/1024 (87%) | 878 (98%) | 15 (2%) | 2 (0%) | 52 | 88 |
| 1 | L | 882/1024 (86%) | 859 (97%) | 21 (2%) | 2 (0%) | 52 | 88 |
| 1 | N | 870/1024 (85%) | 847 (97%) | 20 (2%) | 3 (0%) | 46 | 85 |
| 1 | P | 856/1024 (84%) | 824 (96%) | 31 (4%) | 1 (0%) | 56 | 91 |
| All | All | 7071/8192 (86%) | 6877 (97%) | 184 (3%) | 10 (0%) | 56 | 91 |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L | 93 | VAL |
| 1 | N | 976 | GLU |
| 1 | N | 979 | PRO |
| 1 | K | 568 | LYS |
| 1 | F | 1018 | THR |
| 1 | K | 519 | GLN |
| 1 | D | 519 | GLN |
| 1 | P | 519 | GLN |
| 1 | L | 519 | GLN |
| 1 | N | 947 | HIS |

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 | B | 797/912 (87%) | 668 (84%) | 129 (16%) | 3 | 14 |
| 1 | D | 795/912 (87%) | 678 (85%) | 117 (15%) | 4 | 18 |
| 1 | F | 795/912 (87%) | 679 (85%) | 116 (15%) | 4 | 19 |
| 1 | H | 788/912 (86%) | 665 (84%) | 123 (16%) | 3 | 15 |
| 1 | K | 798/912 (88%) | 668 (84%) | 130 (16%) | 3 | 14 |
| 1 | L | 785/912 (86%) | 663 (84%) | 122 (16%) | 3 | 15 |
| 1 | N | 769/912 (84%) | 642 (84%) | 127 (16%) | 3 | 13 |
| 1 | P | 754/912 (83%) | 626 (83%) | 128 (17%) | 2 | 12 |
| All | All | 6281/7296 (86%) | 5289 (84%) | 992 (16%) | 3 | 15 |

All (992) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 95 | GLU |
| 1 | K | 97 | ASP |
| 1 | K | 108 | LEU |
| 1 | K | 111 | SER |
| 1 | K | 115 | LEU |
| 1 | K | 120 | LEU |
| 1 | K | 133 | THR |
| 1 | K | 138 | ILE |
| 1 | K | 139 | MET |
| 1 | K | 143 | ASP |
| 1 | K | 168 | GLU |
| 1 | K | 171 | SER |
| 1 | K | 175 | LYS |
| 1 | K | 177 | THR |
| 1 | K | 178 | LEU |
| 1 | K | 184 | MET |
| 1 | K | 195 | LYS |
| 1 | K | 206 | ARG |
| 1 | K | 209 | ARG |
| 1 | K | 221 | LEU |
| 1 | K | 223 | ILE |
| 1 | K | 231 | THR |
| 1 | K | 233 | LYS |
| 1 | K | 238 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 256 | GLN |
| 1 | K | 266 | LYS |
| 1 | K | 281 | THR |
| 1 | K | 287 | ILE |
| 1 | K | 288 | ARG |
| 1 | K | 301 | THR |
| 1 | K | 314 | VAL |
| 1 | K | 324 | GLN |
| 1 | K | 335 | MET |
| 1 | K | 337 | THR |
| 1 | K | 359 | GLN |
| 1 | K | 369 | LEU |
| 1 | K | 396 | LEU |
| 1 | K | 404 | HIS |
| 1 | K | 409 | GLU |
| 1 | K | 414 | SER |
| 1 | K | 416 | MET |
| 1 | K | 417 | ASN |
| 1 | K | 418 | GLU |
| 1 | K | 423 | THR |
| 1 | K | 433 | GLN |
| 1 | K | 445 | SER |
| 1 | K | 455 | LEU |
| 1 | K | 463 | GLU |
| 1 | K | 481 | SER |
| 1 | K | 498 | SER |
| 1 | K | 507 | ARG |
| 1 | K | 511 | MET |
| 1 | K | 523 | VAL |
| 1 | K | 525 | LYS |
| 1 | K | 531 | GLN |
| 1 | K | 540 | THR |
| 1 | K | 543 | GLN |
| 1 | K | 553 | SER |
| 1 | K | 563 | SER |
| 1 | K | 569 | SER |
| 1 | K | 571 | LEU |
| 1 | K | 573 | GLN |
| 1 | K | 580 | GLN |
| 1 | K | 583 | SER |
| 1 | K | 589 | GLU |
| 1 | K | 591 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 619 | ARG |
| 1 | K | 621 | THR |
| 1 | K | 647 | ARG |
| 1 | K | 650 | SER |
| 1 | K | 651 | LEU |
| 1 | K | 660 | LYS |
| 1 | K | 664 | VAL |
| 1 | K | 675 | GLN |
| 1 | K | 685 | SER |
| 1 | K | 690 | LEU |
| 1 | K | 692 | LEU |
| 1 | K | 703 | ARG |
| 1 | K | 710 | THR |
| 1 | K | 716 | THR |
| 1 | K | 735 | VAL |
| 1 | K | 743 | ILE |
| 1 | K | 745 | ARG |
| 1 | K | 746 | LEU |
| 1 | K | 749 | GLN |
| 1 | K | 751 | LEU |
| 1 | K | 755 | LEU |
| 1 | K | 756 | ILE |
| 1 | K | 762 | LEU |
| 1 | K | 770 | LEU |
| 1 | K | 788 | ARG |
| 1 | K | 789 | SER |
| 1 | K | 790 | LEU |
| 1 | K | 793 | MET |
| 1 | K | 832 | LEU |
| 1 | K | 847 | LEU |
| 1 | K | 848 | ILE |
| 1 | K | 874 | ARG |
| 1 | K | 878 | LEU |
| 1 | K | 886 | LEU |
| 1 | K | 892 | VAL |
| 1 | K | 896 | LEU |
| 1 | K | 900 | LEU |
| 1 | K | 902 | GLN |
| 1 | K | 909 | LEU |
| 1 | K | 911 | LYS |
| 1 | K | 914 | LEU |
| 1 | K | 918 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | K | 924 | ILE |
| 1 | K | 925 | LYS |
| 1 | K | 926 | SER |
| 1 | K | 934 | ASN |
| 1 | K | 936 | LEU |
| 1 | K | 939 | LEU |
| 1 | K | 966 | GLN |
| 1 | K | 976 | GLU |
| 1 | K | 988 | SER |
| 1 | K | 993 | LYS |
| 1 | K | 995 | THR |
| 1 | K | 996 | LEU |
| 1 | K | 997 | LEU |
| 1 | K | 1003 | THR |
| 1 | K | 1008 | ASP |
| 1 | K | 1010 | TYR |
| 1 | K | 1012 | ILE |
| 1 | K | 1013 | SER |
| 1 | K | 1016 | LYS |
| 1 | K | 1018 | THR |
| 1 | K | 1020 | LYS |
| 1 | K | 1023 | THR |
| 1 | B | 97 | ASP |
| 1 | B | 100 | VAL |
| 1 | B | 115 | LEU |
| 1 | B | 120 | LEU |
| 1 | B | 133 | THR |
| 1 | B | 139 | MET |
| 1 | B | 161 | LEU |
| 1 | B | 168 | GLU |
| 1 | B | 171 | SER |
| 1 | B | 184 | MET |
| 1 | B | 188 | SER |
| 1 | B | 195 | LYS |
| 1 | B | 206 | ARG |
| 1 | B | 209 | ARG |
| 1 | B | 221 | LEU |
| 1 | B | 223 | ILE |
| 1 | B | 225 | ASP |
| 1 | B | 231 | THR |
| 1 | B | 237 | LEU |
| 1 | B | 240 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 256 | GLN |
| 1 | B | 274 | MET |
| 1 | B | 281 | THR |
| 1 | B | 287 | ILE |
| 1 | B | 288 | ARG |
| 1 | B | 314 | VAL |
| 1 | B | 319 | GLU |
| 1 | B | 335 | MET |
| 1 | B | 337 | THR |
| 1 | B | 339 | LEU |
| 1 | B | 352 | GLN |
| 1 | B | 353 | GLU |
| 1 | B | 383 | SER |
| 1 | B | 396 | LEU |
| 1 | B | 409 | GLU |
| 1 | B | 411 | GLU |
| 1 | B | 416 | MET |
| 1 | B | 418 | GLU |
| 1 | B | 421 | LEU |
| 1 | B | 434 | ARG |
| 1 | B | 455 | LEU |
| 1 | B | 463 | GLU |
| 1 | B | 497 | SER |
| 1 | B | 498 | SER |
| 1 | B | 499 | THR |
| 1 | B | 502 | THR |
| 1 | B | 503 | ARG |
| 1 | B | 519 | GLN |
| 1 | B | 523 | VAL |
| 1 | B | 526 | ARG |
| 1 | B | 528 | LEU |
| 1 | B | 529 | TRP |
| 1 | B | 530 | ARG |
| 1 | B | 535 | GLN |
| 1 | B | 540 | THR |
| 1 | B | 541 | THR |
| 1 | B | 542 | GLU |
| 1 | B | 543 | GLN |
| 1 | B | 563 | SER |
| 1 | B | 573 | GLN |
| 1 | B | 583 | SER |
| 1 | B | 588 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 595 | LEU |
| 1 | B | 621 | THR |
| 1 | B | 647 | ARG |
| 1 | B | 662 | LEU |
| 1 | B | 664 | VAL |
| 1 | B | 670 | ASN |
| 1 | B | 685 | SER |
| 1 | B | 689 | ASN |
| 1 | B | 692 | LEU |
| 1 | B | 706 | SER |
| 1 | B | 712 | LYS |
| 1 | B | 713 | ASN |
| 1 | B | 714 | MET |
| 1 | B | 725 | THR |
| 1 | B | 735 | VAL |
| 1 | B | 744 | HIS |
| 1 | B | 749 | GLN |
| 1 | B | 751 | LEU |
| 1 | B | 755 | LEU |
| 1 | B | 762 | LEU |
| 1 | B | 770 | LEU |
| 1 | B | 774 | ARG |
| 1 | B | 789 | SER |
| 1 | B | 790 | LEU |
| 1 | B | 791 | LYS |
| 1 | B | 793 | MET |
| 1 | B | 802 | SER |
| 1 | B | 806 | GLU |
| 1 | B | 822 | LEU |
| 1 | B | 828 | VAL |
| 1 | B | 832 | LEU |
| 1 | B | 847 | LEU |
| 1 | B | 848 | ILE |
| 1 | B | 850 | LEU |
| 1 | B | 851 | SER |
| 1 | B | 857 | GLU |
| 1 | B | 862 | LYS |
| 1 | B | 878 | LEU |
| 1 | B | 880 | GLU |
| 1 | B | 892 | VAL |
| 1 | B | 896 | LEU |
| 1 | B | 900 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 909 | LEU |
| 1 | B | 911 | LYS |
| 1 | B | 914 | LEU |
| 1 | B | 918 | ARG |
| 1 | B | 920 | ARG |
| 1 | B | 924 | ILE |
| 1 | B | 926 | SER |
| 1 | B | 934 | ASN |
| 1 | B | 936 | LEU |
| 1 | B | 939 | LEU |
| 1 | B | 951 | SER |
| 1 | B | 955 | LEU |
| 1 | B | 962 | GLU |
| 1 | B | 964 | LEU |
| 1 | B | 969 | PHE |
| 1 | B | 975 | GLU |
| 1 | B | 988 | SER |
| 1 | B | 989 | GLN |
| 1 | B | 995 | THR |
| 1 | B | 996 | LEU |
| 1 | B | 1002 | LEU |
| 1 | B | 1007 | PHE |
| 1 | B | 1015 | ILE |
| 1 | B | 1018 | THR |
| 1 | B | 1020 | LYS |
| 1 | D | 115 | LEU |
| 1 | D | 120 | LEU |
| 1 | D | 130 | LEU |
| 1 | D | 133 | THR |
| 1 | D | 138 | ILE |
| 1 | D | 139 | MET |
| 1 | D | 142 | LYS |
| 1 | D | 145 | ARG |
| 1 | D | 168 | GLU |
| 1 | D | 181 | ARG |
| 1 | D | 184 | MET |
| 1 | D | 192 | ARG |
| 1 | D | 200 | VAL |
| 1 | D | 206 | ARG |
| 1 | D | 209 | ARG |
| 1 | D | 221 | LEU |
| 1 | D | 227 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 231 | THR |
| 1 | D | 237 | LEU |
| 1 | D | 278 | THR |
| 1 | D | 287 | ILE |
| 1 | D | 288 | ARG |
| 1 | D | 301 | THR |
| 1 | D | 303 | ASP |
| 1 | D | 314 | VAL |
| 1 | D | 334 | LEU |
| 1 | D | 335 | MET |
| 1 | D | 339 | LEU |
| 1 | D | 351 | ARG |
| 1 | D | 352 | GLN |
| 1 | D | 353 | GLU |
| 1 | D | 359 | GLN |
| 1 | D | 371 | ILE |
| 1 | D | 396 | LEU |
| 1 | D | 409 | GLU |
| 1 | D | 411 | GLU |
| 1 | D | 414 | SER |
| 1 | D | 423 | THR |
| 1 | D | 430 | TYR |
| 1 | D | 436 | LYS |
| 1 | D | 445 | SER |
| 1 | D | 455 | LEU |
| 1 | D | 462 | LYS |
| 1 | D | 463 | GLU |
| 1 | D | 475 | ASN |
| 1 | D | 481 | SER |
| 1 | D | 490 | LEU |
| 1 | D | 498 | SER |
| 1 | D | 507 | ARG |
| 1 | D | 511 | MET |
| 1 | D | 523 | VAL |
| 1 | D | 537 | LEU |
| 1 | D | 541 | THR |
| 1 | D | 543 | GLN |
| 1 | D | 547 | LYS |
| 1 | D | 563 | SER |
| 1 | D | 573 | GLN |
| 1 | D | 580 | GLN |
| 1 | D | 583 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 589 | GLU |
| 1 | D | 595 | LEU |
| 1 | D | 614 | LEU |
| 1 | D | 621 | THR |
| 1 | D | 651 | LEU |
| 1 | D | 657 | GLN |
| 1 | D | 664 | VAL |
| 1 | D | 670 | ASN |
| 1 | D | 682 | LYS |
| 1 | D | 685 | SER |
| 1 | D | 689 | ASN |
| 1 | D | 690 | LEU |
| 1 | D | 692 | LEU |
| 1 | D | 696 | ARG |
| 1 | D | 711 | CYS |
| 1 | D | 713 | ASN |
| 1 | D | 725 | THR |
| 1 | D | 730 | GLN |
| 1 | D | 735 | VAL |
| 1 | D | 736 | THR |
| 1 | D | 746 | LEU |
| 1 | D | 755 | LEU |
| 1 | D | 756 | ILE |
| 1 | D | 762 | LEU |
| 1 | D | 770 | LEU |
| 1 | D | 789 | SER |
| 1 | D | 790 | LEU |
| 1 | D | 793 | MET |
| 1 | D | 828 | VAL |
| 1 | D | 832 | LEU |
| 1 | D | 847 | LEU |
| 1 | D | 878 | LEU |
| 1 | D | 886 | LEU |
| 1 | D | 891 | ASP |
| 1 | D | 892 | VAL |
| 1 | D | 900 | LEU |
| 1 | D | 903 | LEU |
| 1 | D | 906 | THR |
| 1 | D | 909 | LEU |
| 1 | D | 914 | LEU |
| 1 | D | 924 | ILE |
| 1 | D | 934 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 936 | LEU |
| 1 | D | 951 | SER |
| 1 | D | 955 | LEU |
| 1 | D | 962 | GLU |
| 1 | D | 964 | LEU |
| 1 | D | 965 | LYS |
| 1 | D | 976 | GLU |
| 1 | D | 978 | LEU |
| 1 | D | 987 | LEU |
| 1 | D | 988 | SER |
| 1 | D | 989 | GLN |
| 1 | D | 993 | LYS |
| 1 | D | 996 | LEU |
| 1 | D | 997 | LEU |
| 1 | D | 1008 | ASP |
| 1 | D | 1018 | THR |
| 1 | F | 97 | ASP |
| 1 | F | 115 | LEU |
| 1 | F | 133 | THR |
| 1 | F | 139 | MET |
| 1 | F | 145 | ARG |
| 1 | F | 161 | LEU |
| 1 | F | 168 | GLU |
| 1 | F | 184 | MET |
| 1 | F | 192 | ARG |
| 1 | F | 205 | LEU |
| 1 | F | 206 | ARG |
| 1 | F | 209 | ARG |
| 1 | F | 219 | GLN |
| 1 | F | 223 | ILE |
| 1 | F | 227 | ILE |
| 1 | F | 231 | THR |
| 1 | F | 239 | LEU |
| 1 | F | 274 | MET |
| 1 | F | 278 | THR |
| 1 | F | 281 | THR |
| 1 | F | 288 | ARG |
| 1 | F | 301 | THR |
| 1 | F | 303 | ASP |
| 1 | F | 308 | LEU |
| 1 | F | 324 | GLN |
| 1 | F | 335 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 337 | THR |
| 1 | F | 339 | LEU |
| 1 | F | 344 | THR |
| 1 | F | 351 | ARG |
| 1 | F | 353 | GLU |
| 1 | F | 357 | HIS |
| 1 | F | 369 | LEU |
| 1 | F | 385 | ASP |
| 1 | F | 389 | SER |
| 1 | F | 396 | LEU |
| 1 | F | 404 | HIS |
| 1 | F | 409 | GLU |
| 1 | F | 415 | SER |
| 1 | F | 423 | THR |
| 1 | F | 433 | GLN |
| 1 | F | 434 | ARG |
| 1 | F | 436 | LYS |
| 1 | F | 455 | LEU |
| 1 | F | 481 | SER |
| 1 | F | 497 | SER |
| 1 | F | 498 | SER |
| 1 | F | 499 | THR |
| 1 | F | 507 | ARG |
| 1 | F | 523 | VAL |
| 1 | F | 540 | THR |
| 1 | F | 543 | GLN |
| 1 | F | 553 | SER |
| 1 | F | 560 | ASN |
| 1 | F | 563 | SER |
| 1 | F | 574 | GLU |
| 1 | F | 580 | GLN |
| 1 | F | 583 | SER |
| 1 | F | 591 | ILE |
| 1 | F | 614 | LEU |
| 1 | F | 619 | ARG |
| 1 | F | 656 | LYS |
| 1 | F | 657 | GLN |
| 1 | F | 664 | VAL |
| 1 | F | 672 | LEU |
| 1 | F | 678 | LYS |
| 1 | F | 682 | LYS |
| 1 | F | 685 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 692 | LEU |
| 1 | F | 710 | THR |
| 1 | F | 715 | HIS |
| 1 | F | 716 | THR |
| 1 | F | 725 | THR |
| 1 | F | 726 | THR |
| 1 | F | 735 | VAL |
| 1 | F | 736 | THR |
| 1 | F | 743 | ILE |
| 1 | F | 746 | LEU |
| 1 | F | 751 | LEU |
| 1 | F | 755 | LEU |
| 1 | F | 756 | ILE |
| 1 | F | 762 | LEU |
| 1 | F | 770 | LEU |
| 1 | F | 788 | ARG |
| 1 | F | 789 | SER |
| 1 | F | 790 | LEU |
| 1 | F | 793 | MET |
| 1 | F | 811 | ILE |
| 1 | F | 813 | LYS |
| 1 | F | 828 | VAL |
| 1 | F | 832 | LEU |
| 1 | F | 847 | LEU |
| 1 | F | 848 | ILE |
| 1 | F | 878 | LEU |
| 1 | F | 891 | ASP |
| 1 | F | 892 | VAL |
| 1 | F | 918 | ARG |
| 1 | F | 922 | GLU |
| 1 | F | 924 | ILE |
| 1 | F | 933 | MET |
| 1 | F | 936 | LEU |
| 1 | F | 951 | SER |
| 1 | F | 962 | GLU |
| 1 | F | 964 | LEU |
| 1 | F | 978 | LEU |
| 1 | F | 983 | LEU |
| 1 | F | 987 | LEU |
| 1 | F | 988 | SER |
| 1 | F | 993 | LYS |
| 1 | F | 995 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | F | 997 | LEU |
| 1 | F | 1003 | THR |
| 1 | F | 1008 | ASP |
| 1 | F | 1015 | ILE |
| 1 | F | 1018 | THR |
| 1 | F | 1023 | THR |
| 1 | H | 103 | GLN |
| 1 | H | 115 | LEU |
| 1 | H | 133 | THR |
| 1 | H | 135 | THR |
| 1 | H | 138 | ILE |
| 1 | H | 139 | MET |
| 1 | H | 143 | ASP |
| 1 | H | 145 | ARG |
| 1 | H | 150 | GLU |
| 1 | H | 154 | LEU |
| 1 | H | 168 | GLU |
| 1 | H | 171 | SER |
| 1 | H | 177 | THR |
| 1 | H | 184 | MET |
| 1 | H | 195 | LYS |
| 1 | H | 205 | LEU |
| 1 | H | 206 | ARG |
| 1 | H | 207 | SER |
| 1 | H | 209 | ARG |
| 1 | H | 220 | LEU |
| 1 | H | 231 | THR |
| 1 | H | 237 | LEU |
| 1 | H | 239 | LEU |
| 1 | H | 254 | HIS |
| 1 | H | 256 | GLN |
| 1 | H | 274 | MET |
| 1 | H | 281 | THR |
| 1 | H | 287 | ILE |
| 1 | H | 289 | HIS |
| 1 | H | 301 | THR |
| 1 | H | 314 | VAL |
| 1 | H | 319 | GLU |
| 1 | H | 324 | GLN |
| 1 | H | 331 | LEU |
| 1 | H | 335 | MET |
| 1 | H | 337 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 339 | LEU |
| 1 | H | 353 | GLU |
| 1 | H | 359 | GLN |
| 1 | H | 385 | ASP |
| 1 | H | 396 | LEU |
| 1 | H | 404 | HIS |
| 1 | H | 405 | LYS |
| 1 | H | 409 | GLU |
| 1 | H | 415 | SER |
| 1 | H | 431 | THR |
| 1 | H | 433 | GLN |
| 1 | H | 440 | LYS |
| 1 | H | 445 | SER |
| 1 | H | 462 | LYS |
| 1 | H | 498 | SER |
| 1 | H | 502 | THR |
| 1 | H | 503 | ARG |
| 1 | H | 518 | LEU |
| 1 | H | 537 | LEU |
| 1 | H | 540 | THR |
| 1 | H | 543 | GLN |
| 1 | H | 551 | VAL |
| 1 | H | 563 | SER |
| 1 | H | 573 | GLN |
| 1 | H | 574 | GLU |
| 1 | H | 583 | SER |
| 1 | H | 591 | ILE |
| 1 | H | 595 | LEU |
| 1 | H | 614 | LEU |
| 1 | H | 615 | ASP |
| 1 | H | 621 | THR |
| 1 | H | 647 | ARG |
| 1 | H | 650 | SER |
| 1 | H | 651 | LEU |
| 1 | H | 664 | VAL |
| 1 | H | 665 | THR |
| 1 | H | 685 | SER |
| 1 | H | 692 | LEU |
| 1 | H | 703 | ARG |
| 1 | H | 710 | THR |
| 1 | H | 713 | ASN |
| 1 | H | 735 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | H | 736 | THR |
| 1 | H | 745 | ARG |
| 1 | H | 746 | LEU |
| 1 | H | 755 | LEU |
| 1 | H | 756 | ILE |
| 1 | H | 762 | LEU |
| 1 | H | 770 | LEU |
| 1 | H | 789 | SER |
| 1 | H | 790 | LEU |
| 1 | H | 793 | MET |
| 1 | H | 818 | GLU |
| 1 | H | 827 | LEU |
| 1 | H | 828 | VAL |
| 1 | H | 832 | LEU |
| 1 | H | 847 | LEU |
| 1 | H | 878 | LEU |
| 1 | H | 890 | TRP |
| 1 | H | 892 | VAL |
| 1 | H | 896 | LEU |
| 1 | H | 900 | LEU |
| 1 | H | 901 | LYS |
| 1 | H | 906 | THR |
| 1 | H | 909 | LEU |
| 1 | H | 914 | LEU |
| 1 | H | 922 | GLU |
| 1 | H | 924 | ILE |
| 1 | H | 926 | SER |
| 1 | H | 934 | ASN |
| 1 | H | 936 | LEU |
| 1 | H | 937 | ARG |
| 1 | H | 959 | ASN |
| 1 | H | 962 | GLU |
| 1 | H | 964 | LEU |
| 1 | H | 988 | SER |
| 1 | H | 993 | LYS |
| 1 | H | 995 | THR |
| 1 | H | 997 | LEU |
| 1 | H | 1002 | LEU |
| 1 | H | 1003 | THR |
| 1 | H | 1008 | ASP |
| 1 | H | 1011 | ASP |
| 1 | H | 1012 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | H | 1015 | ILE |
| 1 | H | 1020 | LYS |
| 1 | H | 1023 | THR |
| 1 | L | 105 | LEU |
| 1 | L | 108 | LEU |
| 1 | L | 115 | LEU |
| 1 | L | 120 | LEU |
| 1 | L | 130 | LEU |
| 1 | L | 133 | THR |
| 1 | L | 138 | ILE |
| 1 | L | 139 | MET |
| 1 | L | 145 | ARG |
| 1 | L | 150 | GLU |
| 1 | L | 154 | LEU |
| 1 | L | 168 | GLU |
| 1 | L | 171 | SER |
| 1 | L | 184 | MET |
| 1 | L | 192 | ARG |
| 1 | L | 195 | LYS |
| 1 | L | 205 | LEU |
| 1 | L | 206 | ARG |
| 1 | L | 207 | SER |
| 1 | L | 209 | ARG |
| 1 | L | 231 | THR |
| 1 | L | 239 | LEU |
| 1 | L | 243 | VAL |
| 1 | L | 288 | ARG |
| 1 | L | 293 | LEU |
| 1 | L | 301 | THR |
| 1 | L | 303 | ASP |
| 1 | L | 314 | VAL |
| 1 | L | 319 | GLU |
| 1 | L | 331 | LEU |
| 1 | L | 335 | MET |
| 1 | L | 339 | LEU |
| 1 | L | 351 | ARG |
| 1 | L | 353 | GLU |
| 1 | L | 359 | GLN |
| 1 | L | 373 | LYS |
| 1 | L | 377 | ARG |
| 1 | L | 385 | ASP |
| 1 | L | 396 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 404 | HIS |
| 1 | L | 405 | LYS |
| 1 | L | 409 | GLU |
| 1 | L | 411 | GLU |
| 1 | L | 431 | THR |
| 1 | L | 436 | LYS |
| 1 | L | 445 | SER |
| 1 | L | 455 | LEU |
| 1 | L | 481 | SER |
| 1 | L | 497 | SER |
| 1 | L | 498 | SER |
| 1 | L | 521 | LEU |
| 1 | L | 522 | SER |
| 1 | L | 532 | GLU |
| 1 | L | 536 | SER |
| 1 | L | 538 | ARG |
| 1 | L | 540 | THR |
| 1 | L | 543 | GLN |
| 1 | L | 560 | ASN |
| 1 | L | 561 | LEU |
| 1 | L | 563 | SER |
| 1 | L | 574 | GLU |
| 1 | L | 580 | GLN |
| 1 | L | 583 | SER |
| 1 | L | 591 | ILE |
| 1 | L | 595 | LEU |
| 1 | L | 621 | THR |
| 1 | L | 647 | ARG |
| 1 | L | 651 | LEU |
| 1 | L | 656 | LYS |
| 1 | L | 657 | GLN |
| 1 | L | 664 | VAL |
| 1 | L | 670 | ASN |
| 1 | L | 685 | SER |
| 1 | L | 692 | LEU |
| 1 | L | 710 | THR |
| 1 | L | 713 | ASN |
| 1 | L | 716 | THR |
| 1 | L | 725 | THR |
| 1 | L | 727 | ASP |
| 1 | L | 735 | VAL |
| 1 | L | 736 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | L | 751 | LEU |
| 1 | L | 755 | LEU |
| 1 | L | 756 | ILE |
| 1 | L | 762 | LEU |
| 1 | L | 770 | LEU |
| 1 | L | 778 | GLU |
| 1 | L | 788 | ARG |
| 1 | L | 789 | SER |
| 1 | L | 790 | LEU |
| 1 | L | 791 | LYS |
| 1 | L | 793 | MET |
| 1 | L | 813 | LYS |
| 1 | L | 828 | VAL |
| 1 | L | 832 | LEU |
| 1 | L | 847 | LEU |
| 1 | L | 848 | ILE |
| 1 | L | 878 | LEU |
| 1 | L | 886 | LEU |
| 1 | L | 890 | TRP |
| 1 | L | 892 | VAL |
| 1 | L | 896 | LEU |
| 1 | L | 900 | LEU |
| 1 | L | 906 | THR |
| 1 | L | 909 | LEU |
| 1 | L | 914 | LEU |
| 1 | L | 922 | GLU |
| 1 | L | 924 | ILE |
| 1 | L | 926 | SER |
| 1 | L | 936 | LEU |
| 1 | L | 939 | LEU |
| 1 | L | 951 | SER |
| 1 | L | 956 | TYR |
| 1 | L | 964 | LEU |
| 1 | L | 965 | LYS |
| 1 | L | 975 | GLU |
| 1 | L | 986 | LYS |
| 1 | L | 988 | SER |
| 1 | L | 995 | THR |
| 1 | L | 996 | LEU |
| 1 | L | 997 | LEU |
| 1 | L | 1023 | THR |
| 1 | N | 96 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 100 | VAL |
| 1 | N | 103 | GLN |
| 1 | N | 108 | LEU |
| 1 | N | 115 | LEU |
| 1 | N | 120 | LEU |
| 1 | N | 133 | THR |
| 1 | N | 138 | ILE |
| 1 | N | 139 | MET |
| 1 | N | 144 | HIS |
| 1 | N | 145 | ARG |
| 1 | N | 150 | GLU |
| 1 | N | 161 | LEU |
| 1 | N | 168 | GLU |
| 1 | N | 171 | SER |
| 1 | N | 177 | THR |
| 1 | N | 184 | MET |
| 1 | N | 195 | LYS |
| 1 | N | 205 | LEU |
| 1 | N | 207 | SER |
| 1 | N | 223 | ILE |
| 1 | N | 231 | THR |
| 1 | N | 239 | LEU |
| 1 | N | 240 | HIS |
| 1 | N | 274 | MET |
| 1 | N | 288 | ARG |
| 1 | N | 301 | THR |
| 1 | N | 303 | ASP |
| 1 | N | 314 | VAL |
| 1 | N | 319 | GLU |
| 1 | N | 324 | GLN |
| 1 | N | 334 | LEU |
| 1 | N | 335 | MET |
| 1 | N | 339 | LEU |
| 1 | N | 353 | GLU |
| 1 | N | 359 | GLN |
| 1 | N | 370 | LEU |
| 1 | N | 396 | LEU |
| 1 | N | 409 | GLU |
| 1 | N | 415 | SER |
| 1 | N | 416 | MET |
| 1 | N | 436 | LYS |
| 1 | N | 455 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 463 | GLU |
| 1 | N | 475 | ASN |
| 1 | N | 480 | ILE |
| 1 | N | 497 | SER |
| 1 | N | 498 | SER |
| 1 | N | 502 | THR |
| 1 | N | 503 | ARG |
| 1 | N | 511 | MET |
| 1 | N | 518 | LEU |
| 1 | N | 523 | VAL |
| 1 | N | 535 | GLN |
| 1 | N | 536 | SER |
| 1 | N | 540 | THR |
| 1 | N | 541 | THR |
| 1 | N | 543 | GLN |
| 1 | N | 551 | VAL |
| 1 | N | 561 | LEU |
| 1 | N | 563 | SER |
| 1 | N | 580 | GLN |
| 1 | N | 583 | SER |
| 1 | N | 591 | ILE |
| 1 | N | 595 | LEU |
| 1 | N | 614 | LEU |
| 1 | N | 621 | THR |
| 1 | N | 647 | ARG |
| 1 | N | 650 | SER |
| 1 | N | 651 | LEU |
| 1 | N | 657 | GLN |
| 1 | N | 660 | LYS |
| 1 | N | 664 | VAL |
| 1 | N | 685 | SER |
| 1 | N | 692 | LEU |
| 1 | N | 725 | THR |
| 1 | N | 735 | VAL |
| 1 | N | 745 | ARG |
| 1 | N | 746 | LEU |
| 1 | N | 751 | LEU |
| 1 | N | 755 | LEU |
| 1 | N | 761 | ASN |
| 1 | N | 762 | LEU |
| 1 | N | 770 | LEU |
| 1 | N | 789 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | N | 790 | LEU |
| 1 | N | 793 | MET |
| 1 | N | 794 | ARG |
| 1 | N | 795 | LEU |
| 1 | N | 802 | SER |
| 1 | N | 809 | ASP |
| 1 | N | 811 | ILE |
| 1 | N | 817 | GLU |
| 1 | N | 818 | GLU |
| 1 | N | 822 | LEU |
| 1 | N | 828 | VAL |
| 1 | N | 832 | LEU |
| 1 | N | 847 | LEU |
| 1 | N | 874 | ARG |
| 1 | N | 878 | LEU |
| 1 | N | 880 | GLU |
| 1 | N | 881 | LEU |
| 1 | N | 886 | LEU |
| 1 | N | 892 | VAL |
| 1 | N | 896 | LEU |
| 1 | N | 900 | LEU |
| 1 | N | 901 | LYS |
| 1 | N | 903 | LEU |
| 1 | N | 914 | LEU |
| 1 | N | 918 | ARG |
| 1 | N | 920 | ARG |
| 1 | N | 924 | ILE |
| 1 | N | 925 | LYS |
| 1 | N | 926 | SER |
| 1 | N | 931 | LEU |
| 1 | N | 936 | LEU |
| 1 | N | 937 | ARG |
| 1 | N | 947 | HIS |
| 1 | N | 955 | LEU |
| 1 | N | 964 | LEU |
| 1 | N | 965 | LYS |
| 1 | N | 975 | GLU |
| 1 | N | 989 | GLN |
| 1 | N | 990 | VAL |
| 1 | N | 993 | LYS |
| 1 | N | 996 | LEU |
| 1 | N | 1003 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 103 | GLN |
| 1 | P | 105 | LEU |
| 1 | P | 115 | LEU |
| 1 | P | 120 | LEU |
| 1 | P | 122 | GLU |
| 1 | P | 130 | LEU |
| 1 | P | 133 | THR |
| 1 | P | 138 | ILE |
| 1 | P | 139 | MET |
| 1 | P | 144 | HIS |
| 1 | P | 145 | ARG |
| 1 | P | 147 | HIS |
| 1 | P | 154 | LEU |
| 1 | P | 161 | LEU |
| 1 | P | 168 | GLU |
| 1 | P | 171 | SER |
| 1 | P | 177 | THR |
| 1 | P | 184 | MET |
| 1 | P | 192 | ARG |
| 1 | P | 195 | LYS |
| 1 | P | 205 | LEU |
| 1 | P | 206 | ARG |
| 1 | P | 207 | SER |
| 1 | P | 209 | ARG |
| 1 | P | 227 | ILE |
| 1 | P | 231 | THR |
| 1 | P | 239 | LEU |
| 1 | P | 243 | VAL |
| 1 | P | 274 | MET |
| 1 | P | 275 | VAL |
| 1 | P | 288 | ARG |
| 1 | P | 301 | THR |
| 1 | P | 314 | VAL |
| 1 | P | 319 | GLU |
| 1 | P | 330 | CYS |
| 1 | P | 334 | LEU |
| 1 | P | 335 | MET |
| 1 | P | 339 | LEU |
| 1 | P | 357 | HIS |
| 1 | P | 359 | GLN |
| 1 | P | 369 | LEU |
| 1 | P | 370 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 377 | ARG |
| 1 | P | 396 | LEU |
| 1 | P | 404 | HIS |
| 1 | P | 409 | GLU |
| 1 | P | 410 | PRO |
| 1 | P | 435 | LEU |
| 1 | P | 436 | LYS |
| 1 | P | 455 | LEU |
| 1 | P | 463 | GLU |
| 1 | P | 498 | SER |
| 1 | P | 503 | ARG |
| 1 | P | 517 | SER |
| 1 | P | 521 | LEU |
| 1 | P | 540 | THR |
| 1 | P | 541 | THR |
| 1 | P | 543 | GLN |
| 1 | P | 551 | VAL |
| 1 | P | 561 | LEU |
| 1 | P | 563 | SER |
| 1 | P | 568 | LYS |
| 1 | P | 569 | SER |
| 1 | P | 580 | GLN |
| 1 | P | 583 | SER |
| 1 | P | 589 | GLU |
| 1 | P | 591 | ILE |
| 1 | P | 595 | LEU |
| 1 | P | 614 | LEU |
| 1 | P | 660 | LYS |
| 1 | P | 662 | LEU |
| 1 | P | 664 | VAL |
| 1 | P | 665 | THR |
| 1 | P | 672 | LEU |
| 1 | P | 674 | LYS |
| 1 | P | 677 | ILE |
| 1 | P | 682 | LYS |
| 1 | P | 685 | SER |
| 1 | P | 689 | ASN |
| 1 | P | 692 | LEU |
| 1 | P | 695 | LYS |
| 1 | P | 703 | ARG |
| 1 | P | 710 | THR |
| 1 | P | 725 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 735 | VAL |
| 1 | P | 746 | LEU |
| 1 | P | 751 | LEU |
| 1 | P | 755 | LEU |
| 1 | P | 756 | ILE |
| 1 | P | 762 | LEU |
| 1 | P | 770 | LEU |
| 1 | P | 788 | ARG |
| 1 | P | 789 | SER |
| 1 | P | 790 | LEU |
| 1 | P | 793 | MET |
| 1 | P | 802 | SER |
| 1 | P | 813 | LYS |
| 1 | P | 827 | LEU |
| 1 | P | 828 | VAL |
| 1 | P | 832 | LEU |
| 1 | P | 847 | LEU |
| 1 | P | 848 | ILE |
| 1 | P | 859 | TYR |
| 1 | P | 861 | GLU |
| 1 | P | 874 | ARG |
| 1 | P | 878 | LEU |
| 1 | P | 892 | VAL |
| 1 | P | 896 | LEU |
| 1 | P | 901 | LYS |
| 1 | P | 906 | THR |
| 1 | P | 909 | LEU |
| 1 | P | 914 | LEU |
| 1 | P | 922 | GLU |
| 1 | P | 924 | ILE |
| 1 | P | 926 | SER |
| 1 | P | 934 | ASN |
| 1 | P | 936 | LEU |
| 1 | P | 951 | SER |
| 1 | P | 955 | LEU |
| 1 | P | 964 | LEU |
| 1 | P | 975 | GLU |
| 1 | P | 980 | ASP |
| 1 | P | 988 | SER |
| 1 | P | 993 | LYS |
| 1 | P | 995 | THR |
| 1 | P | 996 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | P | 997 | LEU |
| 1 | P | 1003 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 289 | HIS |
| 1 | K | 531 | GLN |
| 1 | B | 268 | ASN |
| 1 | B | 552 | ASN |
| 1 | B | 998 | GLN |
| 1 | D | 364 | GLN |
| 1 | D | 573 | GLN |
| 1 | D | 747 | HIS |
| 1 | H | 433 | GLN |
| 1 | H | 715 | HIS |
| 1 | H | 739 | GLN |
| 1 | H | 740 | ASN |
| 1 | L | 324 | GLN |
| 1 | L | 359 | GLN |
| 1 | N | 269 | HIS |
| 1 | N | 657 | GLN |
| 1 | N | 675 | GLN |
| 1 | N | 693 | HIS |
| 1 | N | 761 | ASN |
| 1 | P | 317 | GLN |
| 1 | P | 324 | GLN |
| 1 | P | 359 | GLN |
| 1 | P | 740 | ASN |
| 1 | P | 941 | GLN |
| 1 | P | 947 | HIS |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 1 | SEP | B | 533 | 1 | 8,9,10 | 1.52 | 1 (12%) | 8,12,14 | 1.64 | 1 (12%) |
| 1 | SEP | D | 533 | 1 | 8,9,10 | 1.49 | 1 (12%) | 8,12,14 | 1.77 | 2 (25%) |
| 1 | SEP | F | 533 | 1 | 8,9,10 | 1.49 | 1 (12%) | 8,12,14 | 1.48 | 2 (25%) |
| 1 | SEP | H | 533 | 1 | 8,9,10 | 1.50 | 1 (12%) | 8,12,14 | 1.16 | 1 (12%) |
| 1 | SEP | K | 533 | 1 | 8,9,10 | 1.50 | 1 (12%) | 8,12,14 | 1.57 | 1 (12%) |
| 1 | SEP | L | 533 | 1 | 8,9,10 | 1.50 | 1 (12%) | 8,12,14 | 1.70 | 2 (25%) |
| 1 | SEP | N | 533 | 1 | 4,5,10 | 0.51 | 0 | 2,5,14 | 1.30 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 1 | SEP | B | 533 | 1 | - | 0/6/8/10 | 0/0/0/0 |
| 1 | SEP | D | 533 | 1 | - | 0/6/8/10 | 0/0/0/0 |
| 1 | SEP | F | 533 | 1 | - | 0/6/8/10 | 0/0/0/0 |
| 1 | SEP | H | 533 | 1 | - | 0/6/8/10 | 0/0/0/0 |
| 1 | SEP | K | 533 | 1 | - | 0/6/8/10 | 0/0/0/0 |
| 1 | SEP | L | 533 | 1 | - | 0/6/8/10 | 0/0/0/0 |
| 1 | SEP | N | 533 | 1 | - | 0/2/4/10 | 0/0/0/0 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | F | 533 | SEP | P-O1P | 3.05 | 1.61 | 1.51 |
| 1 | K | 533 | SEP | P-O1P | 3.05 | 1.61 | 1.51 |
| 1 | D | 533 | SEP | P-O1P | 3.09 | 1.61 | 1.51 |
| 1 | B | 533 | SEP | P-O1P | 3.09 | 1.61 | 1.51 |
| 1 | L | 533 | SEP | P-O1P | 3.12 | 1.61 | 1.51 |
| 1 | H | 533 | SEP | P-O1P | 3.12 | 1.61 | 1.51 |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | L | 533 | SEP | O-C-CA | -2.16 | 119.87 | 125.49 |
| 1 | D | 533 | SEP | O-C-CA | -2.04 | 120.17 | 125.49 |
| 1 | F | 533 | SEP | O-C-CA | -2.02 | 120.23 | 125.49 |
| 1 | H | 533 | SEP | OG-CB-CA | 2.02 | 110.00 | 108.27 |
| 1 | F | 533 | SEP | OG-CB-CA | 3.11 | 110.92 | 108.27 |
| 1 | L | 533 | SEP | OG-CB-CA | 3.53 | 111.29 | 108.27 |
| 1 | K | 533 | SEP | OG-CB-CA | 3.65 | 111.39 | 108.27 |
| 1 | B | 533 | SEP | OG-CB-CA | 4.03 | 111.72 | 108.27 |
| 1 | D | 533 | SEP | OG-CB-CA | 4.17 | 111.83 | 108.27 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | B | 533 | SEP | 3 | 0 |
| 1 | F | 533 | SEP | 1 | 0 |
| 1 | H | 533 | SEP | 2 | 0 |
| 1 | K | 533 | SEP | 1 | 0 |

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | ADP | B | 1101 | - | 22,29,29 | 0.99 | 1 (4%) | 27,45,45 | 1.88 | 4 (14%) |
| 3 | SO4 | B | 1102 | - | 4,4,4 | 0.23 | 0 | 6,6,6 | 0.08 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | ADP | D | 1101 | - | 22,29,29 | 1.01 | 1 (4%) | 27,45,45 | 1.84 | 5 (18%) |
| 2 | ADP | F | 1101 | - | 22,29,29 | 0.97 | 1 (4%) | 27,45,45 | 1.83 | 4 (14%) |
| 2 | ADP | H | 1101 | - | 22,29,29 | 0.99 | 1 (4%) | 27,45,45 | 1.85 | 4 (14%) |
| 2 | ADP | K | 1101 | - | 22,29,29 | 1.00 | 1 (4%) | 27,45,45 | 1.92 | 4 (14%) |
| 2 | ADP | L | 1101 | - | 22,29,29 | 1.05 | 1 (4%) | 27,45,45 | 1.66 | 4 (14%) |
| 2 | ADP | N | 1101 | - | 22,29,29 | 1.01 | 1 (4%) | 27,45,45 | 1.89 | 4 (14%) |
| 3 | SO4 | N | 1102 | - | 4,4,4 | 0.23 | 0 | 6,6,6 | 0.09 | 0 |
| 2 | ADP | P | 1101 | - | 22,29,29 | 1.02 | 1 (4%) | 27,45,45 | 1.73 | 4 (14%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 2 | ADP | B | 1101 | - | - | 0/12/32/32 | 0/3/3/3 |
| 3 | SO4 | B | 1102 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | ADP | D | 1101 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | F | 1101 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | H | 1101 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | K | 1101 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | L | 1101 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | N | 1101 | - | - | 0/12/32/32 | 0/3/3/3 |
| 3 | SO4 | N | 1102 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | ADP | P | 1101 | - | - | 0/12/32/32 | 0/3/3/3 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2 | F | 1101 | ADP | C5-C4 | 3.05 | 1.47 | 1.40 |
| 2 | K | 1101 | ADP | C5-C4 | 3.10 | 1.47 | 1.40 |
| 2 | H | 1101 | ADP | C5-C4 | 3.12 | 1.47 | 1.40 |
| 2 | B | 1101 | ADP | C5-C4 | 3.13 | 1.47 | 1.40 |
| 2 | D | 1101 | ADP | C5-C4 | 3.17 | 1.47 | 1.40 |
| 2 | N | 1101 | ADP | C5-C4 | 3.18 | 1.47 | 1.40 |
| 2 | P | 1101 | ADP | C5-C4 | 3.20 | 1.47 | 1.40 |
| 2 | L | 1101 | ADP | C5-C4 | 3.33 | 1.48 | 1.40 |

All (33) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | K | 1101 | ADP | N3-C2-N1 | -6.64 | 123.81 | 128.89 |
| 2 | F | 1101 | ADP | N3-C2-N1 | -6.59 | 123.85 | 128.89 |
| 2 | N | 1101 | ADP | N3-C2-N1 | -6.55 | 123.88 | 128.89 |
| 2 | D | 1101 | ADP | N3-C2-N1 | -6.51 | 123.91 | 128.89 |
| 2 | H | 1101 | ADP | N3-C2-N1 | -6.50 | 123.92 | 128.89 |
| 2 | B | 1101 | ADP | N3-C2-N1 | -6.46 | 123.95 | 128.89 |
| 2 | P | 1101 | ADP | N3-C2-N1 | -6.02 | 124.28 | 128.89 |
| 2 | L | 1101 | ADP | N3-C2-N1 | -5.63 | 124.58 | 128.89 |
| 2 | N | 1101 | ADP | C2'-C1'-N9 | -4.14 | 107.96 | 114.29 |
| 2 | K | 1101 | ADP | PA-O3A-PB | -3.88 | 119.64 | 132.67 |
| 2 | K | 1101 | ADP | C2'-C1'-N9 | -3.83 | 108.44 | 114.29 |
| 2 | H | 1101 | ADP | C2'-C1'-N9 | -3.74 | 108.58 | 114.29 |
| 2 | B | 1101 | ADP | C2'-C1'-N9 | -3.56 | 108.86 | 114.29 |
| 2 | B | 1101 | ADP | PA-O3A-PB | -3.42 | 121.21 | 132.67 |
| 2 | P | 1101 | ADP | PA-O3A-PB | -3.32 | 121.53 | 132.67 |
| 2 | F | 1101 | ADP | PA-O3A-PB | -3.27 | 121.69 | 132.67 |
| 2 | D | 1101 | ADP | PA-O3A-PB | -3.25 | 121.75 | 132.67 |
| 2 | L | 1101 | ADP | PA-O3A-PB | -3.16 | 122.06 | 132.67 |
| 2 | K | 1101 | ADP | C4-C5-N7 | -3.06 | 106.67 | 109.48 |
| 2 | P | 1101 | ADP | C4-C5-N7 | -3.06 | 106.67 | 109.48 |
| 2 | N | 1101 | ADP | C4-C5-N7 | -2.94 | 106.77 | 109.48 |
| 2 | B | 1101 | ADP | C4-C5-N7 | -2.92 | 106.79 | 109.48 |
| 2 | H | 1101 | ADP | PA-O3A-PB | -2.91 | 122.90 | 132.67 |
| 2 | F | 1101 | ADP | C4-C5-N7 | -2.90 | 106.81 | 109.48 |
| 2 | D | 1101 | ADP | C4-C5-N7 | -2.87 | 106.83 | 109.48 |
| 2 | H | 1101 | ADP | C4-C5-N7 | -2.86 | 106.85 | 109.48 |
| 2 | L | 1101 | ADP | C4-C5-N7 | -2.81 | 106.89 | 109.48 |
| 2 | D | 1101 | ADP | C2'-C1'-N9 | -2.75 | 110.09 | 114.29 |
| 2 | F | 1101 | ADP | C2'-C1'-N9 | -2.71 | 110.15 | 114.29 |
| 2 | P | 1101 | ADP | C2'-C1'-N9 | -2.11 | 111.07 | 114.29 |
| 2 | N | 1101 | ADP | PA-O3A-PB | -2.07 | 125.74 | 132.67 |
| 2 | D | 1101 | ADP | C4'-O4'-C1' | 2.05 | 111.97 | 109.72 |
| 2 | L | 1101 | ADP | O4'-C1'-N9 | 2.26 | 112.83 | 108.10 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2 | B | 1101 | ADP | 1 | 0 |
| 2 | D | 1101 | ADP | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2 | F | 1101 | ADP | 1 | 0 |
| 2 | K | 1101 | ADP | 2 | 0 |
| 2 | L | 1101 | ADP | 1 | 0 |
| 2 | P | 1101 | ADP | 2 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|-----------|----|----|-----------------------|-------|
| 1 | B | 902/1024 (88%) | -0.02 | 18 (1%) | 68 | 54 | 3, 15, 68, 143 | 0 |
| 1 | D | 899/1024 (87%) | 0.02 | 27 (3%) | 54 | 39 | 3, 22, 71, 148 | 0 |
| 1 | F | 898/1024 (87%) | 0.01 | 26 (2%) | 55 | 41 | 2, 19, 65, 130 | 0 |
| 1 | H | 897/1024 (87%) | 0.09 | 33 (3%) | 45 | 30 | 4, 17, 61, 155 | 0 |
| 1 | K | 903/1024 (88%) | 0.01 | 21 (2%) | 64 | 49 | 4, 19, 66, 152 | 0 |
| 1 | L | 892/1024 (87%) | -0.00 | 20 (2%) | 65 | 50 | 2, 15, 66, 146 | 0 |
| 1 | N | 881/1024 (86%) | 0.33 | 51 (5%) | 26 | 15 | 4, 41, 106, 178 | 0 |
| 1 | P | 866/1024 (84%) | 0.63 | 103 (11%) | 6 | 3 | 5, 53, 156, 254 | 0 |
| All | All | 7138/8192 (87%) | 0.13 | 299 (4%) | 40 | 26 | 2, 23, 92, 254 | 0 |

All (299) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | H | 1007 | PHE | 7.9 |
| 1 | N | 1021 | LEU | 7.8 |
| 1 | N | 961 | PHE | 6.5 |
| 1 | N | 980 | ASP | 6.4 |
| 1 | P | 987 | LEU | 6.3 |
| 1 | P | 984 | VAL | 6.0 |
| 1 | N | 978 | LEU | 6.0 |
| 1 | N | 979 | PRO | 5.7 |
| 1 | P | 1021 | LEU | 5.7 |
| 1 | H | 712 | LYS | 5.6 |
| 1 | P | 1002 | LEU | 5.6 |
| 1 | H | 1006 | GLU | 5.5 |
| 1 | P | 957 | PHE | 5.5 |
| 1 | B | 1007 | PHE | 5.5 |
| 1 | N | 1015 | ILE | 5.4 |
| 1 | P | 954 | TRP | 5.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | P | 975 | GLU | 5.3 |
| 1 | P | 980 | ASP | 5.3 |
| 1 | P | 1004 | GLY | 5.2 |
| 1 | H | 1011 | ASP | 5.1 |
| 1 | P | 567 | SER | 4.9 |
| 1 | F | 1005 | TRP | 4.9 |
| 1 | N | 1005 | TRP | 4.9 |
| 1 | P | 958 | MET | 4.8 |
| 1 | N | 957 | PHE | 4.8 |
| 1 | P | 955 | LEU | 4.7 |
| 1 | P | 979 | PRO | 4.6 |
| 1 | P | 1005 | TRP | 4.6 |
| 1 | D | 383 | SER | 4.4 |
| 1 | N | 929 | GLU | 4.4 |
| 1 | P | 988 | SER | 4.3 |
| 1 | K | 1006 | GLU | 4.3 |
| 1 | H | 1015 | ILE | 4.3 |
| 1 | P | 985 | ARG | 4.2 |
| 1 | H | 381 | GLY | 4.2 |
| 1 | N | 976 | GLU | 4.2 |
| 1 | N | 975 | GLU | 4.2 |
| 1 | F | 352 | GLN | 4.2 |
| 1 | N | 987 | LEU | 4.2 |
| 1 | L | 987 | LEU | 4.1 |
| 1 | D | 1007 | PHE | 4.1 |
| 1 | P | 961 | PHE | 4.1 |
| 1 | P | 1003 | THR | 4.1 |
| 1 | P | 357 | HIS | 4.1 |
| 1 | P | 863 | ASP | 4.1 |
| 1 | K | 1021 | LEU | 4.1 |
| 1 | L | 378 | TYR | 4.0 |
| 1 | P | 679 | TYR | 4.0 |
| 1 | P | 960 | VAL | 4.0 |
| 1 | F | 1015 | ILE | 4.0 |
| 1 | P | 981 | ALA | 4.0 |
| 1 | K | 1015 | ILE | 3.9 |
| 1 | P | 989 | GLN | 3.9 |
| 1 | N | 712 | LYS | 3.9 |
| 1 | P | 962 | GLU | 3.9 |
| 1 | P | 959 | ASN | 3.9 |
| 1 | P | 974 | THR | 3.8 |
| 1 | P | 982 | ALA | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | P | 704 | LEU | 3.8 |
| 1 | D | 151 | GLN | 3.8 |
| 1 | P | 992 | SER | 3.8 |
| 1 | P | 925 | LYS | 3.8 |
| 1 | B | 353 | GLU | 3.8 |
| 1 | L | 984 | VAL | 3.8 |
| 1 | N | 1000 | VAL | 3.7 |
| 1 | K | 1005 | TRP | 3.7 |
| 1 | P | 670 | ASN | 3.7 |
| 1 | F | 353 | GLU | 3.6 |
| 1 | P | 802 | SER | 3.6 |
| 1 | P | 932 | GLU | 3.6 |
| 1 | P | 708 | LEU | 3.6 |
| 1 | P | 973 | SER | 3.6 |
| 1 | P | 141 | LYS | 3.6 |
| 1 | F | 983 | LEU | 3.5 |
| 1 | P | 331 | LEU | 3.5 |
| 1 | F | 383 | SER | 3.5 |
| 1 | D | 352 | GLN | 3.5 |
| 1 | P | 924 | ILE | 3.5 |
| 1 | D | 323 | ALA | 3.5 |
| 1 | N | 1002 | LEU | 3.4 |
| 1 | N | 821 | ASP | 3.4 |
| 1 | B | 384 | GLY | 3.4 |
| 1 | F | 1007 | PHE | 3.4 |
| 1 | L | 977 | PHE | 3.4 |
| 1 | K | 1023 | THR | 3.4 |
| 1 | D | 353 | GLU | 3.4 |
| 1 | N | 386 | PHE | 3.4 |
| 1 | N | 958 | MET | 3.4 |
| 1 | P | 965 | LYS | 3.3 |
| 1 | B | 352 | GLN | 3.3 |
| 1 | P | 927 | LEU | 3.3 |
| 1 | L | 412 | HIS | 3.3 |
| 1 | N | 952 | ASP | 3.2 |
| 1 | D | 97 | ASP | 3.2 |
| 1 | F | 1006 | GLU | 3.2 |
| 1 | N | 513 | TYR | 3.2 |
| 1 | K | 983 | LEU | 3.2 |
| 1 | P | 783 | LEU | 3.2 |
| 1 | K | 386 | PHE | 3.2 |
| 1 | L | 956 | TYR | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | D | 1023 | THR | 3.2 |
| 1 | F | 151 | GLN | 3.2 |
| 1 | P | 379 | ARG | 3.2 |
| 1 | L | 1005 | TRP | 3.1 |
| 1 | H | 973 | SER | 3.1 |
| 1 | N | 977 | PHE | 3.1 |
| 1 | P | 820 | CYS | 3.1 |
| 1 | L | 431 | THR | 3.1 |
| 1 | N | 670 | ASN | 3.1 |
| 1 | D | 382 | ALA | 3.1 |
| 1 | B | 1023 | THR | 3.0 |
| 1 | F | 386 | PHE | 3.0 |
| 1 | P | 976 | GLU | 3.0 |
| 1 | F | 1023 | THR | 3.0 |
| 1 | P | 991 | LEU | 3.0 |
| 1 | H | 763 | LYS | 3.0 |
| 1 | P | 983 | LEU | 3.0 |
| 1 | P | 355 | GLN | 3.0 |
| 1 | N | 371 | ILE | 3.0 |
| 1 | B | 1005 | TRP | 3.0 |
| 1 | P | 926 | SER | 2.9 |
| 1 | P | 929 | GLU | 2.9 |
| 1 | P | 684 | PHE | 2.9 |
| 1 | B | 524 | THR | 2.9 |
| 1 | D | 1015 | ILE | 2.9 |
| 1 | P | 951 | SER | 2.9 |
| 1 | H | 1022 | VAL | 2.9 |
| 1 | L | 1022 | VAL | 2.9 |
| 1 | N | 378 | TYR | 2.9 |
| 1 | P | 669 | ILE | 2.9 |
| 1 | P | 356 | ALA | 2.9 |
| 1 | H | 388 | ARG | 2.8 |
| 1 | P | 950 | SER | 2.8 |
| 1 | P | 321 | LEU | 2.8 |
| 1 | P | 464 | PRO | 2.8 |
| 1 | P | 455 | LEU | 2.8 |
| 1 | L | 1023 | THR | 2.8 |
| 1 | L | 386 | PHE | 2.8 |
| 1 | L | 983 | LEU | 2.8 |
| 1 | K | 322 | TRP | 2.8 |
| 1 | H | 1009 | ASP | 2.8 |
| 1 | F | 1021 | LEU | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | P | 1019 | PHE | 2.8 |
| 1 | N | 984 | VAL | 2.8 |
| 1 | F | 977 | PHE | 2.8 |
| 1 | K | 1016 | LYS | 2.8 |
| 1 | P | 1000 | VAL | 2.8 |
| 1 | H | 1005 | TRP | 2.7 |
| 1 | H | 977 | PHE | 2.7 |
| 1 | N | 418 | GLU | 2.7 |
| 1 | B | 527 | PRO | 2.7 |
| 1 | P | 152 | LEU | 2.7 |
| 1 | F | 965 | LYS | 2.7 |
| 1 | N | 810 | TYR | 2.7 |
| 1 | N | 988 | SER | 2.7 |
| 1 | P | 672 | LEU | 2.7 |
| 1 | H | 1008 | ASP | 2.7 |
| 1 | H | 378 | TYR | 2.7 |
| 1 | N | 802 | SER | 2.7 |
| 1 | F | 380 | GLY | 2.6 |
| 1 | P | 685 | SER | 2.6 |
| 1 | P | 972 | PHE | 2.6 |
| 1 | B | 378 | TYR | 2.6 |
| 1 | P | 952 | ASP | 2.6 |
| 1 | K | 1007 | PHE | 2.6 |
| 1 | N | 927 | LEU | 2.6 |
| 1 | N | 679 | TYR | 2.6 |
| 1 | P | 764 | ASN | 2.6 |
| 1 | N | 388 | ARG | 2.6 |
| 1 | P | 945 | ALA | 2.6 |
| 1 | D | 431 | THR | 2.6 |
| 1 | H | 1023 | THR | 2.6 |
| 1 | L | 424 | ILE | 2.6 |
| 1 | P | 378 | TYR | 2.6 |
| 1 | H | 951 | SER | 2.6 |
| 1 | D | 327 | GLU | 2.6 |
| 1 | P | 931 | LEU | 2.5 |
| 1 | L | 980 | ASP | 2.5 |
| 1 | H | 1001 | LYS | 2.5 |
| 1 | P | 615 | ASP | 2.5 |
| 1 | H | 1024 | ALA | 2.5 |
| 1 | P | 389 | SER | 2.5 |
| 1 | P | 732 | ILE | 2.5 |
| 1 | K | 617 | TYR | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | D | 302 | GLU | 2.5 |
| 1 | P | 928 | GLY | 2.5 |
| 1 | H | 379 | ARG | 2.5 |
| 1 | K | 981 | ALA | 2.5 |
| 1 | N | 617 | TYR | 2.5 |
| 1 | P | 890 | TRP | 2.5 |
| 1 | N | 357 | HIS | 2.5 |
| 1 | N | 1019 | PHE | 2.5 |
| 1 | F | 994 | LEU | 2.5 |
| 1 | N | 721 | ALA | 2.4 |
| 1 | F | 389 | SER | 2.4 |
| 1 | P | 747 | HIS | 2.4 |
| 1 | N | 822 | LEU | 2.4 |
| 1 | D | 523 | VAL | 2.4 |
| 1 | D | 763 | LYS | 2.4 |
| 1 | P | 996 | LEU | 2.4 |
| 1 | B | 995 | THR | 2.4 |
| 1 | P | 675 | GLN | 2.4 |
| 1 | H | 1012 | ILE | 2.4 |
| 1 | N | 354 | PHE | 2.4 |
| 1 | B | 529 | TRP | 2.4 |
| 1 | P | 683 | ILE | 2.4 |
| 1 | N | 925 | LYS | 2.4 |
| 1 | D | 620 | ALA | 2.4 |
| 1 | K | 380 | GLY | 2.4 |
| 1 | B | 531 | GLN | 2.4 |
| 1 | P | 934 | ASN | 2.3 |
| 1 | N | 762 | LEU | 2.3 |
| 1 | P | 762 | LEU | 2.3 |
| 1 | K | 979 | PRO | 2.3 |
| 1 | H | 380 | GLY | 2.3 |
| 1 | P | 380 | GLY | 2.3 |
| 1 | N | 653 | PHE | 2.3 |
| 1 | N | 981 | ALA | 2.3 |
| 1 | P | 746 | LEU | 2.3 |
| 1 | P | 862 | LYS | 2.3 |
| 1 | D | 379 | ARG | 2.3 |
| 1 | P | 495 | CYS | 2.3 |
| 1 | H | 1004 | GLY | 2.3 |
| 1 | K | 1012 | ILE | 2.3 |
| 1 | N | 761 | ASN | 2.3 |
| 1 | K | 354 | PHE | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | P | 935 | PRO | 2.3 |
| 1 | P | 977 | PHE | 2.3 |
| 1 | L | 979 | PRO | 2.3 |
| 1 | L | 679 | TYR | 2.3 |
| 1 | D | 319 | GLU | 2.3 |
| 1 | F | 378 | TYR | 2.2 |
| 1 | B | 526 | ARG | 2.2 |
| 1 | B | 431 | THR | 2.2 |
| 1 | H | 389 | SER | 2.2 |
| 1 | P | 386 | PHE | 2.2 |
| 1 | H | 269 | HIS | 2.2 |
| 1 | P | 1001 | LYS | 2.2 |
| 1 | D | 414 | SER | 2.2 |
| 1 | P | 716 | THR | 2.2 |
| 1 | F | 1012 | ILE | 2.2 |
| 1 | P | 93 | VAL | 2.2 |
| 1 | K | 1022 | VAL | 2.2 |
| 1 | D | 965 | LYS | 2.2 |
| 1 | H | 1000 | VAL | 2.2 |
| 1 | B | 981 | ALA | 2.2 |
| 1 | F | 357 | HIS | 2.2 |
| 1 | N | 991 | LEU | 2.2 |
| 1 | N | 430 | TYR | 2.2 |
| 1 | K | 976 | GLU | 2.2 |
| 1 | P | 933 | MET | 2.2 |
| 1 | K | 1011 | ASP | 2.2 |
| 1 | P | 707 | VAL | 2.2 |
| 1 | N | 535 | GLN | 2.2 |
| 1 | D | 388 | ARG | 2.2 |
| 1 | L | 976 | GLU | 2.2 |
| 1 | F | 388 | ARG | 2.2 |
| 1 | H | 617 | TYR | 2.2 |
| 1 | P | 715 | HIS | 2.1 |
| 1 | P | 381 | GLY | 2.1 |
| 1 | H | 781 | LYS | 2.1 |
| 1 | F | 985 | ARG | 2.1 |
| 1 | P | 696 | ARG | 2.1 |
| 1 | P | 788 | ARG | 2.1 |
| 1 | D | 966 | GLN | 2.1 |
| 1 | B | 411 | GLU | 2.1 |
| 1 | D | 1006 | GLU | 2.1 |
| 1 | P | 673 | ASN | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | N | 999 | GLU | 2.1 |
| 1 | D | 1010 | TYR | 2.1 |
| 1 | H | 386 | PHE | 2.1 |
| 1 | D | 976 | GLU | 2.1 |
| 1 | H | 980 | ASP | 2.1 |
| 1 | P | 998 | GLN | 2.1 |
| 1 | B | 1024 | ALA | 2.1 |
| 1 | B | 994 | LEU | 2.1 |
| 1 | D | 232 | PHE | 2.1 |
| 1 | H | 978 | LEU | 2.1 |
| 1 | L | 98 | LEU | 2.1 |
| 1 | F | 617 | TYR | 2.1 |
| 1 | H | 976 | GLU | 2.1 |
| 1 | K | 1009 | ASP | 2.1 |
| 1 | F | 322 | TRP | 2.1 |
| 1 | L | 975 | GLU | 2.1 |
| 1 | P | 763 | LYS | 2.1 |
| 1 | K | 987 | LEU | 2.1 |
| 1 | D | 1005 | TRP | 2.1 |
| 1 | N | 809 | ASP | 2.1 |
| 1 | F | 382 | ALA | 2.1 |
| 1 | L | 432 | ALA | 2.1 |
| 1 | N | 98 | LEU | 2.0 |
| 1 | P | 682 | LYS | 2.0 |
| 1 | N | 713 | ASN | 2.0 |
| 1 | N | 804 | ILE | 2.0 |
| 1 | P | 497 | SER | 2.0 |
| 1 | F | 1010 | TYR | 2.0 |
| 1 | P | 786 | GLY | 2.0 |
| 1 | H | 618 | GLU | 2.0 |
| 1 | P | 993 | LYS | 2.0 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 1 | SEP | N | 533 | 6/11 | 0.79 | 0.24 | - | 6,7,16,17 | 0 |
| 1 | SEP | L | 533 | 10/11 | 0.90 | 0.16 | - | 69,69,69,69 | 0 |
| 1 | SEP | B | 533 | 10/11 | 0.83 | 0.22 | - | 54,54,54,54 | 0 |
| 1 | SEP | F | 533 | 10/11 | 0.89 | 0.17 | - | 69,69,69,69 | 0 |
| 1 | SEP | D | 533 | 10/11 | 0.83 | 0.24 | - | 59,59,59,59 | 0 |
| 1 | SEP | K | 533 | 10/11 | 0.92 | 0.15 | - | 67,67,67,68 | 0 |
| 1 | SEP | H | 533 | 10/11 | 0.92 | 0.16 | - | 45,46,46,46 | 0 |

6.3 Carbohydrates [i](#)

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(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 3 | SO4 | B | 1102 | 5/5 | 0.80 | 0.32 | 5.68 | 81,93,103,106 | 0 |
| 2 | ADP | N | 1101 | 27/27 | 0.94 | 0.25 | 0.74 | 9,20,28,39 | 0 |
| 2 | ADP | L | 1101 | 27/27 | 0.94 | 0.25 | 0.65 | 2,4,6,7 | 0 |
| 2 | ADP | B | 1101 | 27/27 | 0.94 | 0.22 | 0.36 | 4,5,7,7 | 0 |
| 2 | ADP | H | 1101 | 27/27 | 0.95 | 0.25 | 0.22 | 4,5,6,8 | 0 |
| 2 | ADP | F | 1101 | 27/27 | 0.95 | 0.21 | 0.00 | 2,2,3,3 | 0 |
| 2 | ADP | K | 1101 | 27/27 | 0.96 | 0.21 | -0.11 | 6,10,15,17 | 0 |
| 2 | ADP | D | 1101 | 27/27 | 0.94 | 0.21 | -0.17 | 3,4,9,10 | 0 |
| 2 | ADP | P | 1101 | 27/27 | 0.95 | 0.23 | -0.25 | 8,18,28,35 | 0 |
| 3 | SO4 | N | 1102 | 5/5 | 0.77 | 0.33 | - | 79,86,87,116 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.