



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 10:10 AM JST

PDB ID : 7D5Z
Title : Crystal structure of EBV gH/gL bound with neutralizing antibody 1D8
Authors : Zhu, Q.; Shan, S.; Yu, J.; Wang, X.; Zhang, L.; Zeng, M.
Deposited on : 2020-09-28
Resolution : 4.20 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

<https://www.wwpdb.org/validation/2017/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:

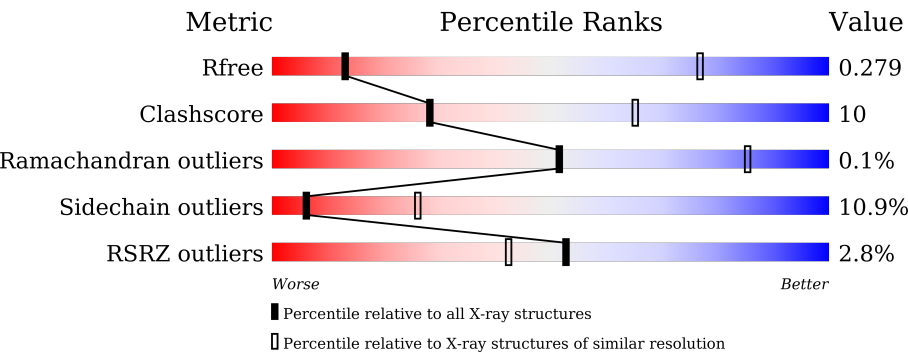
MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

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 4.20 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.



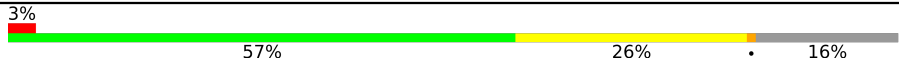







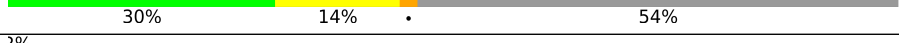

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1005 (4.62-3.78) |
| Clashscore | 141614 | 1044 (4.60-3.80) |
| Ramachandran outliers | 138981 | 1000 (4.60-3.80) |
| Sidechain outliers | 138945 | 1007 (4.62-3.78) |
| RSRZ outliers | 127900 | 1063 (4.70-3.70) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 665 | <div><div>2%</div><div>73%</div><div>23%</div><div>..</div></div> |
| 1 | E | 665 | <div><div>6%</div><div>74%</div><div>22%</div><div>..</div></div> |
| 1 | I | 665 | <div><div>2%</div><div>72%</div><div>24%</div><div>..</div></div> |
| 1 | M | 665 | <div><div>2%</div><div>71%</div><div>24%</div><div>..</div></div> |
| 2 | B | 112 | <div><div>7%</div><div>60%</div><div>22%</div><div>16%</div></div> |
| 2 | F | 112 | <div><div>4%</div><div>56%</div><div>25%</div><div>16%</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | J | 112 |  |
| 2 | N | 112 |  |
| 3 | C | 233 |  |
| 3 | G | 233 |  |
| 3 | K | 233 |  |
| 3 | O | 233 |  |
| 4 | D | 470 |  |
| 4 | H | 470 |  |
| 4 | L | 470 |  |
| 4 | P | 470 |  |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36304 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 Envelope glycoprotein H.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | M | 655 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5099 | 3270 | 842 | 955 | 32 | | | |
| 1 | A | 655 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5099 | 3270 | 842 | 955 | 32 | | | |
| 1 | E | 655 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5099 | 3270 | 842 | 955 | 32 | | | |
| 1 | I | 655 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5099 | 3270 | 842 | 955 | 32 | | | |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| M | 680 | HIS | - | expression tag | UNP Q3KSQ3 |
| M | 681 | HIS | - | expression tag | UNP Q3KSQ3 |
| M | 682 | HIS | - | expression tag | UNP Q3KSQ3 |
| M | 683 | HIS | - | expression tag | UNP Q3KSQ3 |
| M | 684 | HIS | - | expression tag | UNP Q3KSQ3 |
| A | 680 | HIS | - | expression tag | UNP Q3KSQ3 |
| A | 681 | HIS | - | expression tag | UNP Q3KSQ3 |
| A | 682 | HIS | - | expression tag | UNP Q3KSQ3 |
| A | 683 | HIS | - | expression tag | UNP Q3KSQ3 |
| A | 684 | HIS | - | expression tag | UNP Q3KSQ3 |
| E | 680 | HIS | - | expression tag | UNP Q3KSQ3 |
| E | 681 | HIS | - | expression tag | UNP Q3KSQ3 |
| E | 682 | HIS | - | expression tag | UNP Q3KSQ3 |
| E | 683 | HIS | - | expression tag | UNP Q3KSQ3 |
| E | 684 | HIS | - | expression tag | UNP Q3KSQ3 |
| I | 680 | HIS | - | expression tag | UNP Q3KSQ3 |
| I | 681 | HIS | - | expression tag | UNP Q3KSQ3 |
| I | 682 | HIS | - | expression tag | UNP Q3KSQ3 |
| I | 683 | HIS | - | expression tag | UNP Q3KSQ3 |
| I | 684 | HIS | - | expression tag | UNP Q3KSQ3 |

- Molecule 2 is a protein called Envelope glycoprotein L.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | N | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 719 | 454 | 120 | 141 | 4 | | | |
| 2 | B | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 719 | 454 | 120 | 141 | 4 | | | |
| 2 | F | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 719 | 454 | 120 | 141 | 4 | | | |
| 2 | J | 94 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 719 | 454 | 120 | 141 | 4 | | | |

- Molecule 3 is a protein called light chain of 1D8.

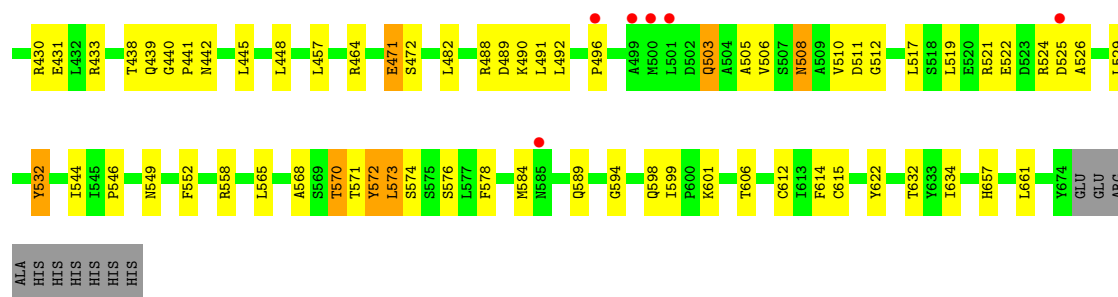
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | O | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1647 | 1035 | 278 | 329 | 5 | | | |
| 3 | C | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1647 | 1035 | 278 | 329 | 5 | | | |
| 3 | G | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1647 | 1035 | 278 | 329 | 5 | | | |
| 3 | K | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1647 | 1035 | 278 | 329 | 5 | | | |

- Molecule 4 is a protein called heavy chain of 1D8.

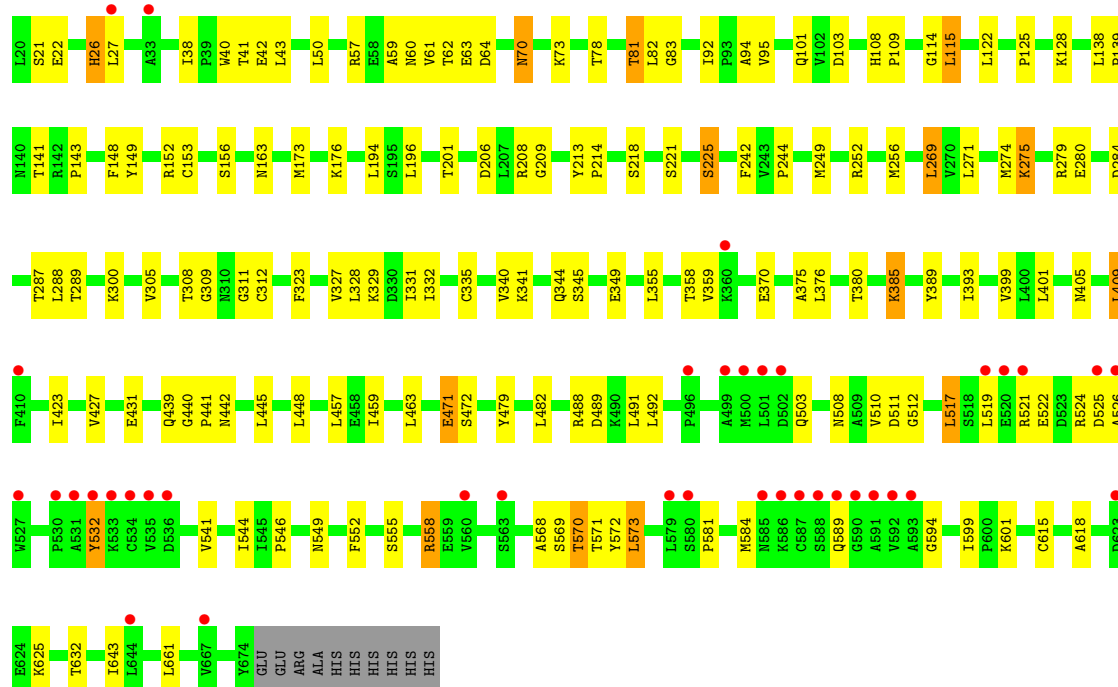
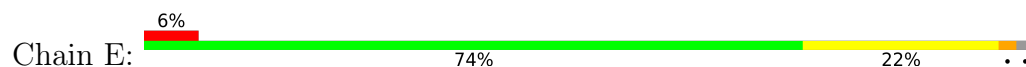
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4 | P | 214 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1611 | 1021 | 273 | 307 | 10 | | | |
| 4 | D | 214 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1611 | 1021 | 273 | 307 | 10 | | | |
| 4 | H | 214 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1611 | 1021 | 273 | 307 | 10 | | | |
| 4 | L | 214 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1611 | 1021 | 273 | 307 | 10 | | | |

- Molecule 1: Envelope glycoprotein H

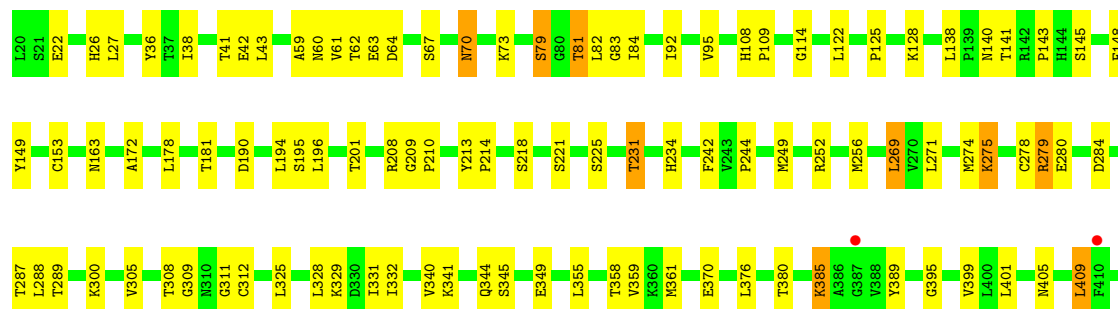


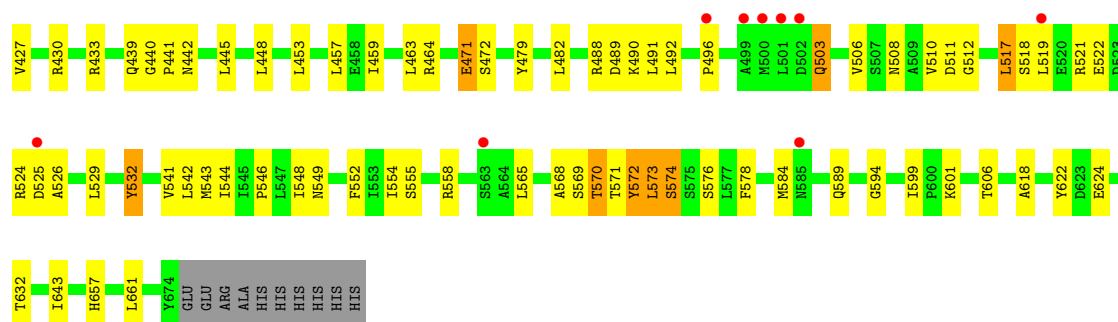


• Molecule 1: Envelope glycoprotein H

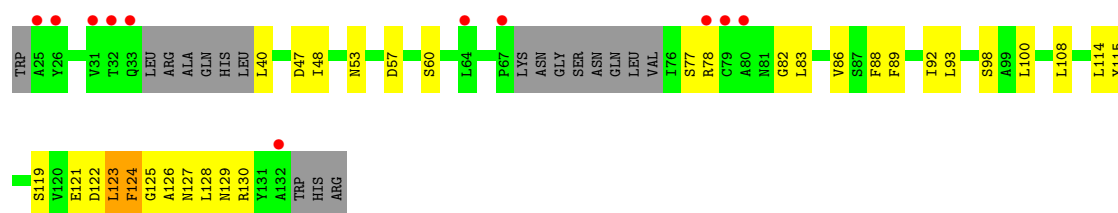


• Molecule 1: Envelope glycoprotein H

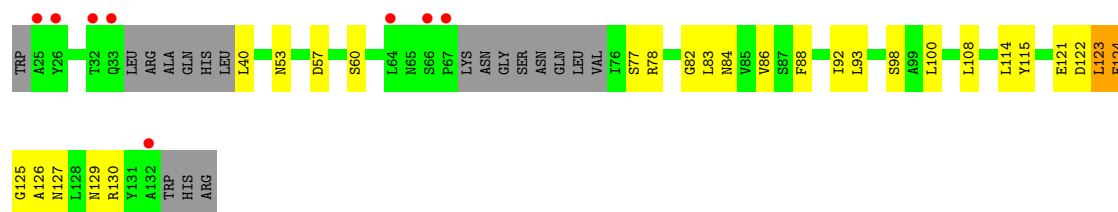




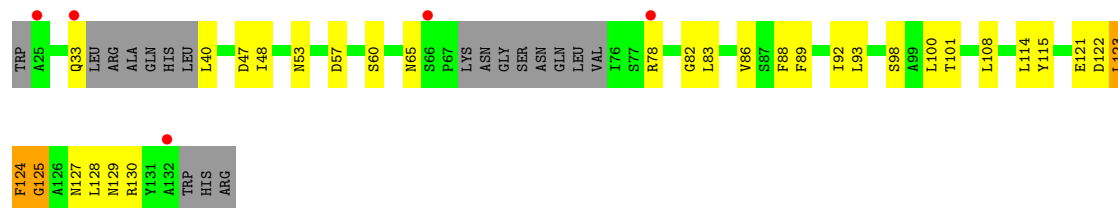
- Molecule 2: Envelope glycoprotein L



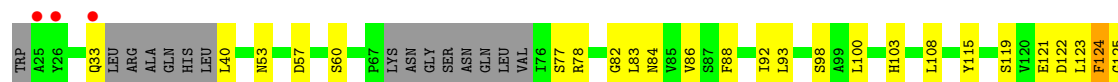
- Molecule 2: Envelope glycoprotein L



- Molecule 2: Envelope glycoprotein L



- Molecule 2: Envelope glycoprotein L



A126
N127
N128
N129
R130
Y131
A132
TRP
HIS
ARG

• Molecule 3: light chain of 1D8

Chain O: 

MET GLY TRP SER CYS ILE LEU PHE LEU VAL ALA THR ALA THR GLY VAL SER D1 I2 T5 Q6 T7 L11 V15 V19 T22 T29 R30 R46 L47 I48 Y49 A50 T53 G64 T72 L73 T74 T75 L78 F83 A84 T85 H91

Y94 P95 W96 Q100 K103 V104 K107 R108 A111 A112 P113 P120 S121 T129 T132 V133 L136 Y140 P141 R142 E143 A144 K145 V146 Q147 W148 L154 D167 D170 S171 T172 L175 S176 L179 E187 E195 V196 T197 H198 L201 P204 V205

T206 E213 CYS

• Molecule 3: light chain of 1D8

Chain C: 

MET GLY TRP SER CYS ILE LEU PHE LEU VAL ALA THR ALA THR GLY VAL SER D1 T5 Q6 T7 L11 V15 R18 V19 T20 L21 T22 T29 R30 W35 P44 K45 R46 L47 I48 A50 T53 L73 T74 T75 L78 F83 A84 T85

H91 Y94 P95 W96 G99 Q100 Q101 K103 I106 K107 R108 A111 A112 P113 S114 V115 S121 T129 V132 V133 C134 L135 L136 Y140 P141 R142 E143 A144 K145 V146 Q147 W148 K149 V150 L154 V163 T164 D167 D170 S171 T172 L175 S176 L179

Y186 E187 Y192 Y196 T197 H198 L201 P204 V205 T206 E213 CYS

• Molecule 3: light chain of 1D8

Chain G: 

MET GLY TRP SER CYS ILE LEU PHE LEU VAL ALA THR ALA THR GLY VAL SER D1 I2 T5 Q6 L11 V15 R18 V19 T29 R30 W35 R46 L47 I48 Y49 A50 A51 S52 T53 D56 G64 T72 L73 T74 T75 L78 F83 A84 T85

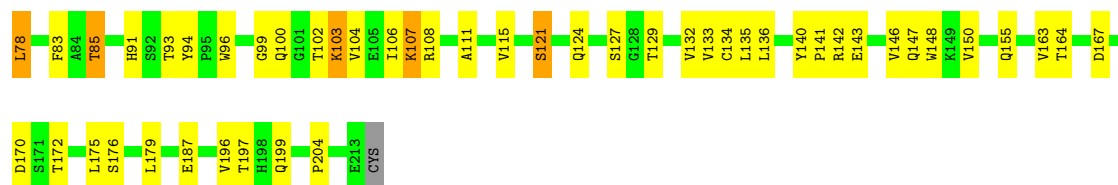
H91 Y94 P95 W96 G99 Q100 K103 V104 K107 R108 A111 A112 P113 S114 V115 S121 T129 V132 V133 C134 L135 L136 Y140 P141 R142 E143 V146 Q147 L154 V163 T164 D167 D170 S171 T172 L175 S176 L179 Y186 E187 Y192

V196 T197 H198 L201 P204 V205 E213 CYS

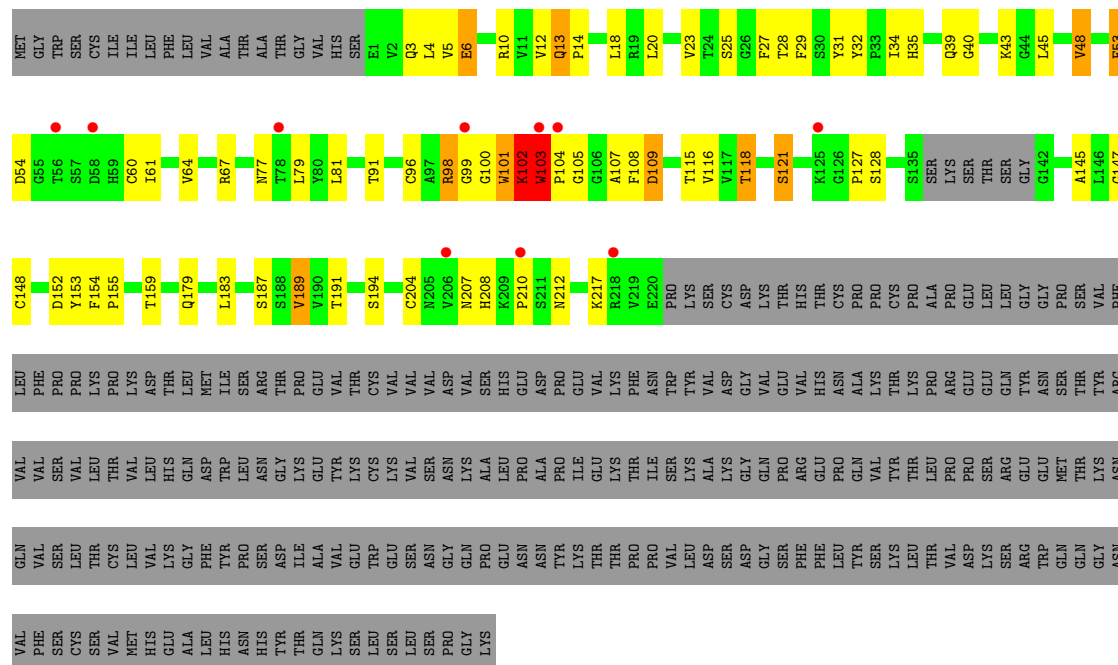
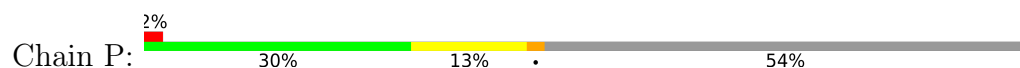
• Molecule 3: light chain of 1D8

Chain K: 

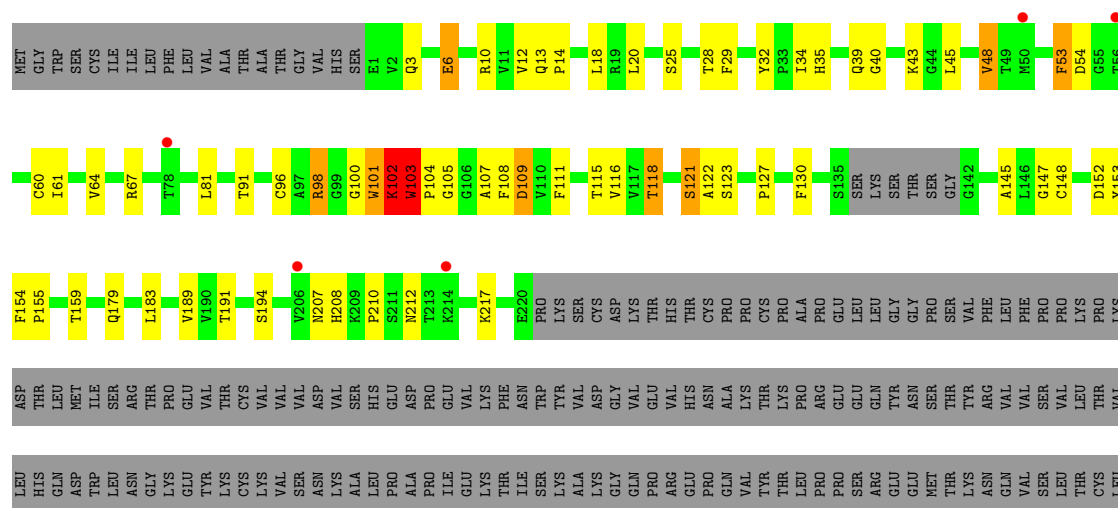
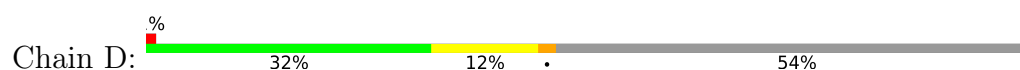
MET GLY TRP SER CYS ILE LEU PHE LEU VAL ALA THR ALA THR GLY VAL SER D1 I2 T5 Q6 T7 L11 V15 R18 V19 T20 T22 T29 R30 P44 R45 R46 L47 I48 Y49 A50 T53 L54 E55 V58 G64 T72 L73 T74 T75



• Molecule 4: heavy chain of 1D8



• Molecule 4: heavy chain of 1D8



PHE
SER
CYS
SER
VAL
MET
HIS
HIS
GLU
ALA
LEU
HIS
HIS
ASN
HIS
TYR
THR
GLN
LYS
SER
LEU
SER
LEU
SER
PRO
GLY
LYS

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 41 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 212.87Å 212.87Å 598.13Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 50.03 – 4.20 50.03 – 4.20 | Depositor EDS |
| % Data completeness (in resolution range) | 99.4 (50.03-4.20) 99.9 (50.03-4.20) | Depositor EDS |
| R_{merge} | 0.13 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.91 (at 4.14Å) | Xtrriage |
| Refinement program | PHENIX 1.18.2_3874 | Depositor |
| R, R_{free} | 0.246 , 0.277 0.250 , 0.279 | Depositor DCC |
| R_{free} test set | 5096 reflections (5.06%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 127.2 | Xtrriage |
| Anisotropy | 0.104 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.33 , 163.9 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$ | Xtrriage |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| F_o, F_c correlation | 0.86 | EDS |
| Total number of atoms | 36304 | wwPDB-VP |
| Average B, all atoms (Å ²) | 153.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1713e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.28 | 0/5208 | 0.50 | 0/7067 |
| 1 | E | 0.28 | 0/5208 | 0.51 | 0/7067 |
| 1 | I | 0.28 | 0/5208 | 0.50 | 0/7067 |
| 1 | M | 0.27 | 0/5208 | 0.50 | 0/7067 |
| 2 | B | 0.28 | 0/729 | 0.49 | 0/987 |
| 2 | F | 0.27 | 0/729 | 0.47 | 0/987 |
| 2 | J | 0.27 | 0/729 | 0.49 | 0/987 |
| 2 | N | 0.27 | 0/729 | 0.47 | 0/987 |
| 3 | C | 0.30 | 0/1686 | 0.52 | 0/2294 |
| 3 | G | 0.29 | 0/1686 | 0.53 | 0/2294 |
| 3 | K | 0.29 | 0/1686 | 0.53 | 0/2294 |
| 3 | O | 0.29 | 0/1686 | 0.53 | 0/2294 |
| 4 | D | 0.32 | 0/1653 | 0.55 | 2/2249 (0.1%) |
| 4 | H | 0.34 | 1/1653 (0.1%) | 0.56 | 2/2249 (0.1%) |
| 4 | L | 0.32 | 0/1653 | 0.56 | 2/2249 (0.1%) |
| 4 | P | 0.31 | 0/1653 | 0.55 | 2/2249 (0.1%) |
| All | All | 0.29 | 1/37104 (0.0%) | 0.51 | 8/50388 (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 |
|-----|-------|---------------------|---------------------|
| 3 | C | 0 | 2 |
| 3 | G | 0 | 1 |
| 3 | K | 0 | 2 |
| 3 | O | 0 | 1 |
| 4 | D | 0 | 2 |
| 4 | H | 0 | 2 |
| 4 | L | 0 | 2 |
| 4 | P | 0 | 2 |
| All | All | 0 | 14 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4 | H | 103 | TRP | CB-CG | 5.80 | 1.60 | 1.50 |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 4 | H | 103 | TRP | N-CA-C | 6.17 | 127.65 | 111.00 |
| 4 | L | 103 | TRP | N-CA-C | 6.09 | 127.44 | 111.00 |
| 4 | L | 102 | LYS | C-N-CA | 6.08 | 136.91 | 121.70 |
| 4 | H | 102 | LYS | C-N-CA | 6.02 | 136.74 | 121.70 |
| 4 | D | 103 | TRP | N-CA-C | 5.90 | 126.93 | 111.00 |
| 4 | P | 103 | TRP | N-CA-C | 5.87 | 126.85 | 111.00 |
| 4 | P | 102 | LYS | C-N-CA | 5.83 | 136.27 | 121.70 |
| 4 | D | 102 | LYS | C-N-CA | 5.82 | 136.25 | 121.70 |

There are no chirality outliers.

All (14) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 3 | C | 106 | ILE | Peptide |
| 3 | C | 29 | ILE | Peptide |
| 4 | D | 102 | LYS | Peptide |
| 4 | D | 121 | SER | Peptide |
| 3 | G | 29 | ILE | Peptide |
| 4 | H | 102 | LYS | Peptide |
| 4 | H | 121 | SER | Peptide |
| 3 | K | 106 | ILE | Peptide |
| 3 | K | 29 | ILE | Peptide |
| 4 | L | 102 | LYS | Peptide |
| 4 | L | 121 | SER | Peptide |
| 3 | O | 29 | ILE | Peptide |
| 4 | P | 102 | LYS | Peptide |
| 4 | P | 121 | SER | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 5099 | 0 | 5119 | 91 | 0 |
| 1 | E | 5099 | 0 | 5119 | 87 | 0 |
| 1 | I | 5099 | 0 | 5119 | 99 | 0 |
| 1 | M | 5099 | 0 | 5119 | 102 | 0 |
| 2 | B | 719 | 0 | 703 | 15 | 0 |
| 2 | F | 719 | 0 | 703 | 19 | 0 |
| 2 | J | 719 | 0 | 703 | 19 | 0 |
| 2 | N | 719 | 0 | 703 | 18 | 0 |
| 3 | C | 1647 | 0 | 1598 | 37 | 0 |
| 3 | G | 1647 | 0 | 1598 | 36 | 0 |
| 3 | K | 1647 | 0 | 1598 | 38 | 0 |
| 3 | O | 1647 | 0 | 1598 | 29 | 0 |
| 4 | D | 1611 | 0 | 1568 | 43 | 0 |
| 4 | H | 1611 | 0 | 1568 | 45 | 0 |
| 4 | L | 1611 | 0 | 1568 | 47 | 0 |
| 4 | P | 1611 | 0 | 1568 | 54 | 0 |
| All | All | 36304 | 0 | 35952 | 708 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (708) 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:M:201:THR:HG22 | 1:M:225:SER:HB2 | 1.53 | 0.88 |
| 3:K:75:ILE:HG12 | 3:K:78:LEU:HD23 | 1.59 | 0.84 |
| 1:I:201:THR:HG22 | 1:I:225:SER:HB2 | 1.59 | 0.84 |
| 1:I:526:ALA:HB1 | 1:I:532:TYR:HE2 | 1.44 | 0.82 |
| 3:G:75:ILE:HG12 | 3:G:78:LEU:HD23 | 1.62 | 0.81 |
| 1:A:201:THR:HG22 | 1:A:225:SER:HB2 | 1.62 | 0.81 |
| 3:C:75:ILE:HG12 | 3:C:78:LEU:HD23 | 1.63 | 0.80 |
| 1:A:81:THR:HG21 | 2:J:125:GLY:HA2 | 1.62 | 0.78 |
| 1:M:81:THR:HG21 | 2:F:125:GLY:HA2 | 1.66 | 0.78 |
| 2:B:125:GLY:HA2 | 1:I:81:THR:HG21 | 1.68 | 0.76 |
| 1:A:526:ALA:HB1 | 1:A:532:TYR:HE2 | 1.52 | 0.74 |
| 1:E:114:GLY:HA2 | 1:E:358:THR:HG21 | 1.69 | 0.74 |
| 1:I:570:THR:OG1 | 1:I:571:THR:N | 2.20 | 0.74 |
| 1:E:141:THR:HG23 | 1:E:143:PRO:HD2 | 1.70 | 0.74 |
| 2:N:125:GLY:HA2 | 1:E:81:THR:HG21 | 1.70 | 0.73 |
| 1:A:570:THR:OG1 | 1:A:571:THR:N | 2.19 | 0.73 |
| 1:I:114:GLY:HA2 | 1:I:358:THR:HG21 | 1.71 | 0.73 |
| 1:M:526:ALA:HB1 | 1:M:532:TYR:HE2 | 1.54 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:114:GLY:HA2 | 1:A:358:THR:HG21 | 1.71 | 0.72 |
| 1:E:60:ASN:HB3 | 1:E:63:GLU:HB2 | 1.71 | 0.72 |
| 1:M:448:LEU:HD13 | 1:M:546:PRO:HD2 | 1.72 | 0.72 |
| 1:E:526:ALA:HB1 | 1:E:532:TYR:HE2 | 1.55 | 0.71 |
| 4:L:20:LEU:HD12 | 4:L:81:LEU:HD23 | 1.71 | 0.71 |
| 1:A:448:LEU:HD13 | 1:A:546:PRO:HD2 | 1.72 | 0.71 |
| 1:A:60:ASN:HB3 | 1:A:63:GLU:HB2 | 1.73 | 0.71 |
| 1:M:570:THR:OG1 | 1:M:571:THR:N | 2.22 | 0.71 |
| 1:E:522:GLU:HG3 | 1:E:524:ARG:HG2 | 1.72 | 0.70 |
| 2:J:93:LEU:HB2 | 2:J:108:LEU:HD13 | 1.74 | 0.70 |
| 3:C:108:ARG:HH22 | 3:C:111:ALA:HB3 | 1.58 | 0.69 |
| 1:M:114:GLY:HA2 | 1:M:358:THR:HG21 | 1.74 | 0.69 |
| 1:E:570:THR:OG1 | 1:E:571:THR:N | 2.23 | 0.69 |
| 1:M:522:GLU:HG3 | 1:M:524:ARG:HG2 | 1.74 | 0.69 |
| 4:D:20:LEU:HD12 | 4:D:81:LEU:HD23 | 1.75 | 0.69 |
| 1:E:201:THR:HG22 | 1:E:225:SER:HB2 | 1.73 | 0.69 |
| 1:M:82:LEU:HG | 1:M:83:GLY:H | 1.58 | 0.69 |
| 3:O:75:ILE:HG12 | 3:O:78:LEU:HD23 | 1.74 | 0.69 |
| 1:I:122:LEU:HA | 1:I:312:CYS:HA | 1.75 | 0.69 |
| 1:I:448:LEU:HD13 | 1:I:546:PRO:HD2 | 1.75 | 0.68 |
| 1:M:60:ASN:HB3 | 1:M:63:GLU:HB2 | 1.75 | 0.68 |
| 1:E:122:LEU:HA | 1:E:312:CYS:HA | 1.76 | 0.68 |
| 1:A:122:LEU:HA | 1:A:312:CYS:HA | 1.76 | 0.68 |
| 1:I:269:LEU:HD12 | 1:I:331:ILE:HG23 | 1.75 | 0.68 |
| 2:B:60:SER:HB3 | 2:B:83:LEU:HG | 1.76 | 0.67 |
| 3:C:197:THR:HG23 | 3:C:204:PRO:HG3 | 1.76 | 0.67 |
| 1:I:565:LEU:HD11 | 1:I:578:PHE:HB3 | 1.75 | 0.67 |
| 2:N:60:SER:HB3 | 2:N:83:LEU:HG | 1.77 | 0.67 |
| 4:P:14:PRO:HD2 | 4:P:121:SER:HB3 | 1.75 | 0.67 |
| 1:M:275:LYS:HE2 | 1:M:512:GLY:HA3 | 1.77 | 0.66 |
| 2:B:93:LEU:HB2 | 2:B:108:LEU:HD13 | 1.78 | 0.66 |
| 3:K:197:THR:HG23 | 3:K:204:PRO:HG3 | 1.77 | 0.66 |
| 1:A:522:GLU:HG3 | 1:A:524:ARG:HG2 | 1.77 | 0.66 |
| 1:E:482:LEU:HD22 | 1:E:544:ILE:HB | 1.78 | 0.66 |
| 1:I:60:ASN:HB3 | 1:I:63:GLU:HB2 | 1.77 | 0.65 |
| 1:M:122:LEU:HA | 1:M:312:CYS:HA | 1.79 | 0.65 |
| 2:F:93:LEU:HB2 | 2:F:108:LEU:HD13 | 1.79 | 0.65 |
| 4:H:20:LEU:HD12 | 4:H:81:LEU:HD23 | 1.79 | 0.65 |
| 1:E:526:ALA:HB1 | 1:E:532:TYR:CE2 | 2.31 | 0.65 |
| 1:M:401:LEU:O | 1:M:405:ASN:ND2 | 2.30 | 0.64 |
| 3:O:108:ARG:HH22 | 3:O:111:ALA:HB3 | 1.62 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:269:LEU:HD12 | 1:M:331:ILE:HG23 | 1.80 | 0.64 |
| 1:I:522:GLU:HG3 | 1:I:524:ARG:HG2 | 1.79 | 0.64 |
| 2:N:121:GLU:HB3 | 2:F:121:GLU:HB3 | 1.79 | 0.64 |
| 1:E:541:VAL:HA | 1:E:555:SER:HB3 | 1.80 | 0.64 |
| 4:P:40:GLY:HA3 | 4:P:43:LYS:HE3 | 1.80 | 0.63 |
| 2:N:93:LEU:HB2 | 2:N:108:LEU:HD13 | 1.78 | 0.63 |
| 2:J:60:SER:HB3 | 2:J:83:LEU:HG | 1.78 | 0.63 |
| 1:I:82:LEU:HG | 1:I:83:GLY:H | 1.63 | 0.63 |
| 1:E:279:ARG:HG3 | 1:E:280:GLU:H | 1.64 | 0.63 |
| 4:D:39:GLN:HB2 | 4:D:45:LEU:HD23 | 1.80 | 0.63 |
| 1:I:526:ALA:HB1 | 1:I:532:TYR:CE2 | 2.30 | 0.63 |
| 4:L:53:PHE:CD1 | 4:L:103:TRP:HB2 | 2.33 | 0.63 |
| 1:A:275:LYS:HE2 | 1:A:512:GLY:HA3 | 1.81 | 0.63 |
| 2:F:60:SER:HB3 | 2:F:83:LEU:HG | 1.79 | 0.63 |
| 3:K:108:ARG:HH22 | 3:K:111:ALA:HB3 | 1.63 | 0.63 |
| 1:M:242:PHE:CZ | 1:M:244:PRO:HG3 | 2.34 | 0.62 |
| 1:M:526:ALA:HB1 | 1:M:532:TYR:CE2 | 2.33 | 0.62 |
| 1:A:82:LEU:HG | 1:A:83:GLY:H | 1.64 | 0.62 |
| 4:P:20:LEU:HD12 | 4:P:81:LEU:HD23 | 1.81 | 0.62 |
| 1:A:565:LEU:HD11 | 1:A:578:PHE:HB3 | 1.82 | 0.62 |
| 4:D:127:PRO:HB3 | 4:D:153:TYR:HB3 | 1.82 | 0.62 |
| 4:D:14:PRO:HD2 | 4:D:121:SER:HB3 | 1.82 | 0.61 |
| 4:D:53:PHE:CD1 | 4:D:103:TRP:HB2 | 2.35 | 0.61 |
| 1:I:242:PHE:CZ | 1:I:244:PRO:HG3 | 2.35 | 0.61 |
| 1:E:82:LEU:HG | 1:E:83:GLY:H | 1.66 | 0.61 |
| 3:O:19:VAL:HB | 3:O:75:ILE:HG23 | 1.83 | 0.61 |
| 1:A:526:ALA:HB1 | 1:A:532:TYR:CE2 | 2.33 | 0.61 |
| 2:B:125:GLY:HA2 | 1:I:81:THR:CG2 | 2.30 | 0.61 |
| 1:E:448:LEU:HD13 | 1:E:546:PRO:HD2 | 1.83 | 0.61 |
| 1:M:81:THR:CG2 | 2:F:125:GLY:HA2 | 2.30 | 0.60 |
| 3:K:146:VAL:HG22 | 3:K:196:VAL:HG22 | 1.83 | 0.60 |
| 4:H:53:PHE:CD1 | 4:H:103:TRP:HB2 | 2.36 | 0.60 |
| 1:A:81:THR:CG2 | 2:J:125:GLY:HA2 | 2.31 | 0.60 |
| 1:I:279:ARG:HG3 | 1:I:280:GLU:H | 1.67 | 0.60 |
| 4:D:91:THR:HG23 | 4:D:118:THR:HA | 1.83 | 0.60 |
| 1:E:488:ARG:NH1 | 1:E:511:ASP:OD1 | 2.35 | 0.59 |
| 1:A:269:LEU:HD12 | 1:A:331:ILE:HG23 | 1.83 | 0.59 |
| 4:L:40:GLY:HA3 | 4:L:43:LYS:HE3 | 1.83 | 0.59 |
| 4:L:91:THR:HG23 | 4:L:118:THR:HA | 1.84 | 0.59 |
| 4:P:53:PHE:CD1 | 4:P:103:TRP:HB2 | 2.36 | 0.59 |
| 4:H:40:GLY:HA3 | 4:H:43:LYS:HE3 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:401:LEU:O | 1:I:405:ASN:ND2 | 2.35 | 0.59 |
| 1:A:279:ARG:HG3 | 1:A:280:GLU:H | 1.65 | 0.59 |
| 1:E:138:LEU:HD13 | 1:E:148:PHE:HB3 | 1.84 | 0.59 |
| 1:I:482:LEU:HD22 | 1:I:544:ILE:HB | 1.82 | 0.59 |
| 4:L:127:PRO:HB3 | 4:L:153:TYR:HB3 | 1.85 | 0.59 |
| 1:A:401:LEU:O | 1:A:405:ASN:ND2 | 2.36 | 0.59 |
| 4:P:127:PRO:HB3 | 4:P:153:TYR:HB3 | 1.84 | 0.59 |
| 1:E:275:LYS:HE2 | 1:E:512:GLY:HA3 | 1.83 | 0.59 |
| 1:A:209:GLY:O | 2:B:115:TYR:OH | 2.21 | 0.58 |
| 4:L:20:LEU:HB2 | 4:L:81:LEU:HB3 | 1.85 | 0.58 |
| 1:M:138:LEU:HD13 | 1:M:148:PHE:HB3 | 1.84 | 0.58 |
| 1:M:279:ARG:HG3 | 1:M:280:GLU:H | 1.68 | 0.58 |
| 1:M:86:LEU:N | 1:M:221:SER:OG | 2.34 | 0.58 |
| 3:K:132:VAL:HB | 3:K:179:LEU:HB3 | 1.86 | 0.58 |
| 4:P:39:GLN:HB2 | 4:P:45:LEU:HD23 | 1.85 | 0.58 |
| 1:A:138:LEU:HD13 | 1:A:148:PHE:HB3 | 1.84 | 0.58 |
| 1:I:311:GLY:HA2 | 4:L:101:TRP:CE3 | 2.38 | 0.58 |
| 3:O:132:VAL:HB | 3:O:179:LEU:HB3 | 1.86 | 0.58 |
| 1:A:242:PHE:CZ | 1:A:244:PRO:HG3 | 2.39 | 0.58 |
| 1:E:573:LEU:HD13 | 1:E:625:LYS:HG2 | 1.86 | 0.58 |
| 3:K:85:THR:HA | 3:K:103:LYS:HA | 1.85 | 0.58 |
| 4:L:208:HIS:CD2 | 4:L:210:PRO:HD2 | 2.39 | 0.58 |
| 1:M:82:LEU:CG | 1:M:83:GLY:H | 2.16 | 0.57 |
| 1:I:503:GLN:HA | 1:I:506:VAL:HB | 1.85 | 0.57 |
| 4:P:91:THR:HG23 | 4:P:118:THR:HA | 1.87 | 0.57 |
| 1:A:311:GLY:HA2 | 4:D:101:TRP:CE3 | 2.38 | 0.57 |
| 2:N:125:GLY:HA2 | 1:E:81:THR:CG2 | 2.33 | 0.57 |
| 4:P:208:HIS:CD2 | 4:P:210:PRO:HD2 | 2.39 | 0.57 |
| 1:A:568:ALA:HA | 1:A:599:ILE:HD13 | 1.85 | 0.57 |
| 1:A:482:LEU:HD22 | 1:A:544:ILE:HB | 1.85 | 0.57 |
| 4:D:152:ASP:OD1 | 4:D:179:GLN:NE2 | 2.38 | 0.57 |
| 1:E:70:ASN:HA | 1:E:73:LYS:HE3 | 1.86 | 0.57 |
| 1:I:568:ALA:HA | 1:I:599:ILE:HD13 | 1.87 | 0.57 |
| 4:H:208:HIS:CD2 | 4:H:210:PRO:HD2 | 2.40 | 0.56 |
| 4:H:14:PRO:HD2 | 4:H:121:SER:HB3 | 1.85 | 0.56 |
| 1:M:311:GLY:HA2 | 4:P:101:TRP:CE3 | 2.39 | 0.56 |
| 1:A:589:GLN:H | 1:A:589:GLN:CD | 2.09 | 0.56 |
| 1:E:242:PHE:CZ | 1:E:244:PRO:HG3 | 2.40 | 0.56 |
| 1:E:632:THR:HG21 | 1:E:643:ILE:HD11 | 1.87 | 0.56 |
| 3:G:197:THR:HG23 | 3:G:204:PRO:HG3 | 1.86 | 0.56 |
| 4:D:159:THR:HB | 4:D:207:ASN:HB3 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:19:VAL:HB | 3:C:75:ILE:HG23 | 1.88 | 0.56 |
| 1:I:571:THR:HG23 | 1:I:574:SER:H | 1.70 | 0.56 |
| 4:D:152:ASP:HB3 | 4:D:183:LEU:HD13 | 1.88 | 0.56 |
| 1:I:138:LEU:HD13 | 1:I:148:PHE:HB3 | 1.86 | 0.56 |
| 3:C:108:ARG:CZ | 3:C:172:THR:HG22 | 2.36 | 0.56 |
| 4:H:91:THR:HG23 | 4:H:118:THR:HA | 1.88 | 0.56 |
| 4:L:147:GLY:HA3 | 4:L:189:VAL:HG12 | 1.88 | 0.56 |
| 3:K:50:ALA:HB3 | 3:K:53:THR:HG23 | 1.88 | 0.56 |
| 4:H:61:ILE:HG22 | 4:H:64:VAL:HG22 | 1.87 | 0.55 |
| 1:M:572:TYR:CE1 | 1:A:170:THR:HG21 | 2.41 | 0.55 |
| 1:M:482:LEU:HD22 | 1:M:544:ILE:HB | 1.87 | 0.55 |
| 4:H:127:PRO:HB3 | 4:H:153:TYR:HB3 | 1.88 | 0.55 |
| 4:P:32:TYR:HE1 | 4:P:101:TRP:HD1 | 1.53 | 0.55 |
| 1:I:92:ILE:O | 4:L:102:LYS:HD3 | 2.07 | 0.55 |
| 1:I:275:LYS:HE2 | 1:I:512:GLY:HA3 | 1.88 | 0.55 |
| 4:L:34:ILE:HG22 | 4:L:35:HIS:N | 2.21 | 0.55 |
| 3:K:108:ARG:CZ | 3:K:172:THR:HG22 | 2.36 | 0.55 |
| 3:C:132:VAL:HB | 3:C:179:LEU:HB3 | 1.89 | 0.54 |
| 4:L:39:GLN:HB2 | 4:L:45:LEU:HD23 | 1.89 | 0.54 |
| 4:L:152:ASP:OD1 | 4:L:179:GLN:NE2 | 2.38 | 0.54 |
| 4:D:208:HIS:CD2 | 4:D:210:PRO:HD2 | 2.41 | 0.54 |
| 1:I:64:ASP:N | 1:I:64:ASP:OD1 | 2.40 | 0.54 |
| 1:A:64:ASP:OD1 | 1:A:64:ASP:N | 2.40 | 0.54 |
| 1:M:568:ALA:HA | 1:M:599:ILE:HD13 | 1.90 | 0.54 |
| 1:I:70:ASN:HA | 1:I:73:LYS:HE3 | 1.89 | 0.54 |
| 1:A:380:THR:HG22 | 1:A:427:VAL:HG22 | 1.90 | 0.54 |
| 1:M:589:GLN:CD | 1:M:589:GLN:H | 2.11 | 0.54 |
| 3:O:108:ARG:CZ | 3:O:172:THR:HG22 | 2.37 | 0.54 |
| 1:E:279:ARG:HG3 | 1:E:280:GLU:N | 2.24 | 0.53 |
| 1:E:401:LEU:O | 1:E:405:ASN:ND2 | 2.40 | 0.53 |
| 3:G:50:ALA:HB3 | 3:G:53:THR:HG23 | 1.91 | 0.53 |
| 4:D:20:LEU:HB2 | 4:D:81:LEU:HB3 | 1.91 | 0.53 |
| 1:M:464:ARG:HB2 | 1:M:496:PRO:HG3 | 1.90 | 0.53 |
| 3:G:108:ARG:CZ | 3:G:172:THR:HG22 | 2.38 | 0.53 |
| 1:M:448:LEU:HD22 | 1:M:546:PRO:O | 2.09 | 0.53 |
| 1:A:385:LYS:HG2 | 1:A:385:LYS:O | 2.09 | 0.53 |
| 2:B:57:ASP:HB3 | 2:B:130:ARG:NH2 | 2.24 | 0.53 |
| 1:A:503:GLN:HA | 1:A:506:VAL:HB | 1.91 | 0.53 |
| 4:D:32:TYR:HE1 | 4:D:101:TRP:HD1 | 1.55 | 0.53 |
| 4:P:6:GLU:HG2 | 4:P:96:CYS:SG | 2.48 | 0.52 |
| 1:E:269:LEU:HD12 | 1:E:331:ILE:HG23 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:622:TYR:CE1 | 1:I:657:HIS:HB2 | 2.44 | 0.52 |
| 1:E:82:LEU:CG | 1:E:83:GLY:H | 2.22 | 0.52 |
| 1:E:311:GLY:HA2 | 4:H:101:TRP:CE3 | 2.44 | 0.52 |
| 1:I:385:LYS:O | 1:I:385:LYS:HG2 | 2.08 | 0.52 |
| 1:E:393:ILE:HG12 | 1:E:431:GLU:HG3 | 1.91 | 0.52 |
| 1:I:140:ASN:HA | 1:I:145:SER:HB3 | 1.91 | 0.52 |
| 1:I:589:GLN:H | 1:I:589:GLN:CD | 2.11 | 0.52 |
| 1:A:249:MET:SD | 1:A:289:THR:HG23 | 2.50 | 0.52 |
| 3:C:50:ALA:HB3 | 3:C:53:THR:HG23 | 1.91 | 0.52 |
| 1:I:210:PRO:HB3 | 2:J:83:LEU:HD13 | 1.90 | 0.52 |
| 4:H:6:GLU:HG3 | 4:H:113:PRO:HD2 | 1.91 | 0.52 |
| 1:I:284:ASP:OD1 | 1:I:287:THR:OG1 | 2.25 | 0.52 |
| 3:G:19:VAL:HB | 3:G:75:ILE:HG23 | 1.92 | 0.52 |
| 1:I:92:ILE:HB | 4:L:102:LYS:HE2 | 1.91 | 0.52 |
| 3:C:91:HIS:HB2 | 3:C:96:TRP:CZ2 | 2.45 | 0.52 |
| 1:M:140:ASN:HA | 1:M:145:SER:HB3 | 1.91 | 0.52 |
| 4:P:101:TRP:HZ2 | 4:P:107:ALA:HB3 | 1.74 | 0.52 |
| 4:P:152:ASP:HA | 4:P:183:LEU:HB3 | 1.92 | 0.52 |
| 4:D:64:VAL:HA | 4:D:67:ARG:HH11 | 1.74 | 0.51 |
| 1:A:488:ARG:NH1 | 1:A:511:ASP:OD1 | 2.42 | 0.51 |
| 3:G:94:TYR:HB3 | 3:G:96:TRP:CD1 | 2.46 | 0.51 |
| 1:I:82:LEU:CG | 1:I:83:GLY:H | 2.23 | 0.51 |
| 4:L:152:ASP:HB3 | 4:L:183:LEU:HD13 | 1.91 | 0.51 |
| 1:M:503:GLN:HA | 1:M:506:VAL:HB | 1.91 | 0.51 |
| 2:J:57:ASP:HB3 | 2:J:130:ARG:NH2 | 2.26 | 0.51 |
| 1:E:92:ILE:O | 4:H:102:LYS:HD3 | 2.11 | 0.51 |
| 1:M:64:ASP:OD1 | 1:M:64:ASP:N | 2.43 | 0.51 |
| 4:H:34:ILE:HG22 | 4:H:35:HIS:N | 2.26 | 0.51 |
| 1:M:92:ILE:O | 4:P:102:LYS:HD3 | 2.11 | 0.51 |
| 1:A:59:ALA:HB1 | 2:B:84:ASN:HB3 | 1.93 | 0.51 |
| 4:P:20:LEU:HB2 | 4:P:81:LEU:HB3 | 1.93 | 0.51 |
| 1:E:115:LEU:HD11 | 1:E:375:ALA:HB2 | 1.92 | 0.51 |
| 4:L:34:ILE:CG2 | 4:L:35:HIS:N | 2.74 | 0.51 |
| 1:M:385:LYS:O | 1:M:385:LYS:HG2 | 2.09 | 0.51 |
| 4:L:173:THR:HG23 | 4:L:188:SER:HB2 | 1.91 | 0.50 |
| 3:O:140:TYR:CG | 3:O:141:PRO:HA | 2.45 | 0.50 |
| 1:I:309:GLY:HA3 | 4:L:32:TYR:OH | 2.12 | 0.50 |
| 4:P:64:VAL:HA | 4:P:67:ARG:HH11 | 1.75 | 0.50 |
| 1:A:82:LEU:CG | 1:A:83:GLY:H | 2.23 | 0.50 |
| 1:A:491:LEU:HB2 | 1:A:510:VAL:HG13 | 1.92 | 0.50 |
| 1:M:571:THR:HG23 | 1:M:573:LEU:H | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:57:ASP:HB3 | 2:N:130:ARG:NH2 | 2.26 | 0.50 |
| 2:N:124:PHE:C | 2:N:126:ALA:H | 2.15 | 0.50 |
| 1:E:94:ALA:HB1 | 4:H:104:PRO:HD3 | 1.92 | 0.50 |
| 3:G:85:THR:HA | 3:G:103:LYS:HA | 1.92 | 0.50 |
| 1:M:82:LEU:CD2 | 2:F:129:ASN:H | 2.25 | 0.50 |
| 1:M:181:THR:HG23 | 1:M:195:SER:HB3 | 1.94 | 0.50 |
| 1:M:558:ARG:NH2 | 1:M:594:GLY:O | 2.44 | 0.50 |
| 3:O:94:TYR:HB3 | 3:O:96:TRP:CD1 | 2.47 | 0.50 |
| 3:O:198:HIS:HB3 | 3:O:201:LEU:HG | 1.92 | 0.50 |
| 4:D:61:ILE:HG22 | 4:D:64:VAL:HG22 | 1.92 | 0.50 |
| 1:E:558:ARG:NH2 | 1:E:594:GLY:O | 2.44 | 0.50 |
| 1:I:488:ARG:NH1 | 1:I:511:ASP:OD1 | 2.44 | 0.50 |
| 3:K:136:LEU:HB2 | 3:K:175:LEU:HB3 | 1.94 | 0.50 |
| 4:L:14:PRO:HD2 | 4:L:121:SER:HB3 | 1.93 | 0.50 |
| 1:A:86:LEU:N | 1:A:221:SER:OG | 2.38 | 0.50 |
| 4:H:152:ASP:HB3 | 4:H:183:LEU:HD13 | 1.94 | 0.50 |
| 1:A:140:ASN:HA | 1:A:145:SER:HB3 | 1.94 | 0.50 |
| 3:C:21:LEU:HD22 | 3:C:102:THR:HG21 | 1.94 | 0.50 |
| 1:I:491:LEU:HB2 | 1:I:510:VAL:HG13 | 1.94 | 0.50 |
| 1:A:558:ARG:NH2 | 1:A:594:GLY:O | 2.44 | 0.49 |
| 1:I:548:ILE:O | 1:I:549:ASN:HB2 | 2.12 | 0.49 |
| 4:L:159:THR:HB | 4:L:207:ASN:HB3 | 1.93 | 0.49 |
| 1:A:571:THR:HG23 | 1:A:573:LEU:H | 1.77 | 0.49 |
| 2:F:57:ASP:HB3 | 2:F:130:ARG:NH2 | 2.26 | 0.49 |
| 2:B:82:GLY:O | 2:B:86:VAL:HG23 | 2.12 | 0.49 |
| 4:D:103:TRP:CD1 | 4:D:104:PRO:HD3 | 2.47 | 0.49 |
| 2:B:121:GLU:HB3 | 2:J:121:GLU:HB3 | 1.94 | 0.49 |
| 1:E:249:MET:SD | 1:E:289:THR:HG23 | 2.53 | 0.49 |
| 3:G:108:ARG:HH22 | 3:G:111:ALA:HB3 | 1.76 | 0.49 |
| 4:H:32:TYR:HE1 | 4:H:101:TRP:HD1 | 1.59 | 0.49 |
| 1:I:209:GLY:O | 2:J:115:TYR:OH | 2.24 | 0.49 |
| 1:I:542:LEU:HB2 | 1:I:554:ILE:HG22 | 1.94 | 0.49 |
| 3:C:146:VAL:HG22 | 3:C:196:VAL:HG22 | 1.95 | 0.49 |
| 4:D:147:GLY:HA3 | 4:D:189:VAL:HG12 | 1.94 | 0.49 |
| 4:H:147:GLY:HA3 | 4:H:189:VAL:HG12 | 1.94 | 0.49 |
| 3:C:94:TYR:HB3 | 3:C:96:TRP:CD1 | 2.48 | 0.49 |
| 4:P:152:ASP:OD1 | 4:P:179:GLN:NE2 | 2.45 | 0.49 |
| 4:D:100:GLY:HA2 | 4:D:105:GLY:O | 2.12 | 0.49 |
| 1:E:305:VAL:O | 1:E:308:THR:HG22 | 2.13 | 0.49 |
| 4:P:12:VAL:HG11 | 4:P:18:LEU:HB2 | 1.94 | 0.49 |
| 1:E:479:TYR:HA | 1:E:517:LEU:HD23 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:11:LEU:HD22 | 3:G:104:VAL:HG22 | 1.95 | 0.49 |
| 1:I:305:VAL:O | 1:I:308:THR:HG22 | 2.12 | 0.49 |
| 1:M:232:PHE:HE1 | 1:E:73:LYS:HD3 | 1.76 | 0.48 |
| 1:E:385:LYS:O | 1:E:385:LYS:HG2 | 2.12 | 0.48 |
| 4:H:152:ASP:OD1 | 4:H:179:GLN:NE2 | 2.46 | 0.48 |
| 1:A:448:LEU:HD22 | 1:A:546:PRO:O | 2.14 | 0.48 |
| 3:G:136:LEU:HD13 | 3:G:175:LEU:HD22 | 1.94 | 0.48 |
| 4:P:100:GLY:HA2 | 4:P:105:GLY:O | 2.13 | 0.48 |
| 1:A:305:VAL:O | 1:A:308:THR:HG22 | 2.14 | 0.48 |
| 2:B:88:PHE:O | 2:B:92:ILE:HG12 | 2.13 | 0.48 |
| 1:E:491:LEU:HB2 | 1:E:510:VAL:HG13 | 1.96 | 0.48 |
| 1:M:565:LEU:HD11 | 1:M:578:PHE:HB3 | 1.96 | 0.48 |
| 4:P:13:GLN:HG3 | 4:P:121:SER:HB3 | 1.95 | 0.48 |
| 3:K:91:HIS:HB2 | 3:K:96:TRP:CZ2 | 2.49 | 0.48 |
| 1:I:141:THR:HG23 | 1:I:143:PRO:HD2 | 1.95 | 0.48 |
| 3:C:136:LEU:HD13 | 3:C:175:LEU:HD22 | 1.95 | 0.48 |
| 1:I:448:LEU:HD22 | 1:I:546:PRO:O | 2.14 | 0.48 |
| 3:K:140:TYR:CG | 3:K:141:PRO:HA | 2.49 | 0.48 |
| 1:M:284:ASP:OD1 | 1:M:287:THR:OG1 | 2.28 | 0.48 |
| 3:O:46:ARG:HG2 | 4:P:109:ASP:HA | 1.95 | 0.48 |
| 3:O:48:ILE:HD12 | 3:O:73:LEU:HD12 | 1.96 | 0.48 |
| 4:D:152:ASP:HA | 4:D:183:LEU:HB3 | 1.95 | 0.48 |
| 1:E:128:LYS:NZ | 3:G:56:ASP:OD1 | 2.36 | 0.48 |
| 2:N:123:LEU:HD13 | 2:N:123:LEU:HA | 1.72 | 0.47 |
| 3:O:91:HIS:HB2 | 3:O:96:TRP:CZ2 | 2.48 | 0.47 |
| 4:P:103:TRP:CD1 | 4:P:104:PRO:HD3 | 2.49 | 0.47 |
| 1:E:309:GLY:HA3 | 4:H:32:TYR:OH | 2.14 | 0.47 |
| 2:F:82:GLY:O | 2:F:86:VAL:HG23 | 2.14 | 0.47 |
| 3:K:11:LEU:HD22 | 3:K:104:VAL:HG22 | 1.96 | 0.47 |
| 1:M:572:TYR:CG | 1:M:572:TYR:O | 2.67 | 0.47 |
| 3:O:136:LEU:HD13 | 3:O:175:LEU:HD22 | 1.95 | 0.47 |
| 1:A:231:THR:HB | 1:A:234:HIS:H | 1.78 | 0.47 |
| 2:B:124:PHE:C | 2:B:126:ALA:H | 2.17 | 0.47 |
| 3:C:30:ARG:H | 3:C:30:ARG:HG3 | 1.48 | 0.47 |
| 1:M:141:THR:HG23 | 1:M:143:PRO:HD2 | 1.96 | 0.47 |
| 1:M:305:VAL:O | 1:M:308:THR:HG22 | 2.14 | 0.47 |
| 2:N:82:GLY:O | 2:N:86:VAL:HG23 | 2.14 | 0.47 |
| 4:P:152:ASP:HB3 | 4:P:183:LEU:HD13 | 1.97 | 0.47 |
| 1:A:430:ARG:HA | 1:A:433:ARG:HG3 | 1.97 | 0.47 |
| 1:E:92:ILE:HB | 4:H:102:LYS:HE2 | 1.97 | 0.47 |
| 1:M:376:LEU:HD11 | 1:M:399:VAL:HG21 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:380:THR:HG22 | 1:M:427:VAL:HG22 | 1.97 | 0.47 |
| 3:C:85:THR:HA | 3:C:103:LYS:HA | 1.96 | 0.47 |
| 1:E:108:HIS:ND1 | 1:E:109:PRO:HD2 | 2.30 | 0.47 |
| 4:H:178:LEU:HD12 | 4:H:184:TYR:CZ | 2.49 | 0.47 |
| 3:O:146:VAL:HG22 | 3:O:196:VAL:HG22 | 1.96 | 0.47 |
| 4:P:61:ILE:HG22 | 4:P:64:VAL:HG22 | 1.95 | 0.47 |
| 3:K:48:ILE:HD12 | 3:K:73:LEU:HD12 | 1.97 | 0.47 |
| 1:M:622:TYR:CE1 | 1:M:657:HIS:HB2 | 2.50 | 0.47 |
| 3:O:11:LEU:HD22 | 3:O:104:VAL:HG22 | 1.97 | 0.47 |
| 3:O:85:THR:HA | 3:O:103:LYS:HA | 1.96 | 0.47 |
| 4:P:4:LEU:HD11 | 4:P:98:ARG:HG2 | 1.97 | 0.47 |
| 1:A:214:PRO:O | 2:J:125:GLY:HA3 | 2.14 | 0.47 |
| 1:A:464:ARG:HB2 | 1:A:496:PRO:HG3 | 1.97 | 0.47 |
| 3:C:140:TYR:CG | 3:C:141:PRO:HA | 2.49 | 0.47 |
| 4:D:34:ILE:HG22 | 4:D:35:HIS:N | 2.29 | 0.47 |
| 4:D:145:ALA:HB2 | 4:D:191:THR:HG22 | 1.96 | 0.47 |
| 1:E:448:LEU:HD22 | 1:E:546:PRO:O | 2.14 | 0.47 |
| 3:G:18:ARG:HH11 | 3:G:18:ARG:HB2 | 1.80 | 0.47 |
| 3:G:201:LEU:HD13 | 3:G:205:VAL:HG23 | 1.95 | 0.47 |
| 1:I:618:ALA:HB3 | 1:I:661:LEU:HB2 | 1.97 | 0.47 |
| 3:K:94:TYR:HB3 | 3:K:96:TRP:CD1 | 2.50 | 0.47 |
| 3:G:132:VAL:HB | 3:G:179:LEU:HB3 | 1.96 | 0.47 |
| 3:O:136:LEU:HB2 | 3:O:175:LEU:HB3 | 1.96 | 0.47 |
| 3:G:46:ARG:HG2 | 4:H:109:ASP:HA | 1.97 | 0.47 |
| 3:O:113:PRO:HD3 | 3:O:198:HIS:ND1 | 2.30 | 0.47 |
| 3:C:167:ASP:HB3 | 3:C:170:ASP:OD1 | 2.15 | 0.47 |
| 4:H:34:ILE:CG2 | 4:H:35:HIS:N | 2.77 | 0.47 |
| 2:J:88:PHE:O | 2:J:92:ILE:HG12 | 2.15 | 0.47 |
| 3:K:7:THR:HG23 | 3:K:22:THR:HB | 1.96 | 0.47 |
| 1:M:78:THR:HB | 1:M:81:THR:HB | 1.97 | 0.46 |
| 1:M:271:LEU:O | 1:M:275:LYS:HD2 | 2.15 | 0.46 |
| 1:E:26:HIS:HE2 | 2:F:47:ASP:HB3 | 1.80 | 0.46 |
| 1:E:380:THR:HG22 | 1:E:427:VAL:HG22 | 1.97 | 0.46 |
| 2:N:129:ASN:H | 1:E:82:LEU:CD2 | 2.29 | 0.46 |
| 4:P:34:ILE:HG22 | 4:P:35:HIS:N | 2.31 | 0.46 |
| 4:P:10:ARG:HB2 | 4:P:18:LEU:HD21 | 1.98 | 0.46 |
| 1:A:409:LEU:H | 1:A:409:LEU:HG | 1.36 | 0.46 |
| 1:A:571:THR:HG23 | 1:A:574:SER:H | 1.80 | 0.46 |
| 1:I:125:PRO:HA | 1:I:128:LYS:HE2 | 1.96 | 0.46 |
| 3:K:6:GLN:HG3 | 3:K:99:GLY:HA3 | 1.96 | 0.46 |
| 1:M:549:ASN:HA | 1:M:584:MET:SD | 2.56 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:88:PHE:O | 2:N:92:ILE:HG12 | 2.14 | 0.46 |
| 2:N:125:GLY:HA3 | 1:E:214:PRO:O | 2.15 | 0.46 |
| 3:C:48:ILE:HD12 | 3:C:73:LEU:HD12 | 1.98 | 0.46 |
| 1:I:380:THR:HG22 | 1:I:427:VAL:HG22 | 1.96 | 0.46 |
| 4:L:61:ILE:HG22 | 4:L:64:VAL:HG22 | 1.96 | 0.46 |
| 4:L:211:SER:OG | 4:L:213:THR:OG1 | 2.25 | 0.46 |
| 1:A:284:ASP:OD1 | 1:A:287:THR:OG1 | 2.29 | 0.46 |
| 3:C:46:ARG:HG2 | 4:D:109:ASP:HA | 1.98 | 0.46 |
| 1:E:62:THR:HB | 2:F:33:GLN:HA | 1.97 | 0.46 |
| 4:L:12:VAL:HG11 | 4:L:18:LEU:HB2 | 1.97 | 0.46 |
| 4:P:102:LYS:HB2 | 4:P:102:LYS:HE3 | 1.85 | 0.46 |
| 4:H:53:PHE:HB3 | 4:H:103:TRP:HB3 | 1.97 | 0.46 |
| 3:K:64:GLY:HA2 | 3:K:72:THR:O | 2.16 | 0.46 |
| 3:K:163:VAL:HG12 | 3:K:164:THR:O | 2.15 | 0.46 |
| 4:L:145:ALA:HB2 | 4:L:191:THR:HG22 | 1.97 | 0.46 |
| 3:O:167:ASP:HB3 | 3:O:170:ASP:OD1 | 2.16 | 0.46 |
| 1:A:82:LEU:CD2 | 2:J:129:ASN:H | 2.28 | 0.46 |
| 1:A:279:ARG:HG3 | 1:A:280:GLU:N | 2.30 | 0.46 |
| 1:A:311:GLY:HA3 | 4:D:101:TRP:HB2 | 1.97 | 0.46 |
| 1:A:505:ALA:HA | 1:A:508:ASN:HB2 | 1.97 | 0.46 |
| 4:D:53:PHE:HB3 | 4:D:103:TRP:CB | 2.45 | 0.46 |
| 1:I:570:THR:HG1 | 1:I:571:THR:H | 1.62 | 0.46 |
| 1:M:279:ARG:HG3 | 1:M:280:GLU:N | 2.31 | 0.46 |
| 2:N:122:ASP:HA | 2:N:124:PHE:CE1 | 2.51 | 0.46 |
| 4:P:29:PHE:HE1 | 4:P:34:ILE:HD11 | 1.81 | 0.46 |
| 1:E:209:GLY:O | 2:F:115:TYR:OH | 2.32 | 0.46 |
| 1:E:618:ALA:HB3 | 1:E:661:LEU:HB2 | 1.98 | 0.46 |
| 3:K:136:LEU:HD13 | 3:K:175:LEU:HD22 | 1.96 | 0.46 |
| 1:M:94:ALA:HB1 | 4:P:104:PRO:HD3 | 1.97 | 0.46 |
| 1:M:618:ALA:HB3 | 1:M:661:LEU:HB2 | 1.98 | 0.46 |
| 1:E:328:LEU:HG | 1:E:332:ILE:HD12 | 1.98 | 0.46 |
| 1:I:275:LYS:HE3 | 1:I:275:LYS:N | 2.30 | 0.46 |
| 4:L:32:TYR:HE1 | 4:L:101:TRP:HD1 | 1.64 | 0.46 |
| 1:A:572:TYR:CG | 1:A:572:TYR:O | 2.69 | 0.45 |
| 2:B:129:ASN:H | 1:I:82:LEU:CD2 | 2.29 | 0.45 |
| 3:C:113:PRO:HD3 | 3:C:198:HIS:ND1 | 2.31 | 0.45 |
| 3:G:140:TYR:CG | 3:G:141:PRO:HA | 2.50 | 0.45 |
| 4:H:12:VAL:HG11 | 4:H:18:LEU:HB2 | 1.97 | 0.45 |
| 1:I:376:LEU:HD11 | 1:I:399:VAL:HG21 | 1.98 | 0.45 |
| 1:M:249:MET:SD | 1:M:289:THR:HG23 | 2.56 | 0.45 |
| 3:O:107:LYS:HG3 | 3:O:108:ARG:N | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:P:5:VAL:O | 4:P:23:VAL:N | 2.34 | 0.45 |
| 4:P:29:PHE:CE1 | 4:P:34:ILE:HD11 | 2.50 | 0.45 |
| 1:I:328:LEU:HG | 1:I:332:ILE:HD12 | 1.98 | 0.45 |
| 1:I:376:LEU:O | 1:I:380:THR:HG23 | 2.17 | 0.45 |
| 2:J:82:GLY:O | 2:J:86:VAL:HG23 | 2.17 | 0.45 |
| 4:P:98:ARG:HG3 | 4:P:109:ASP:OD1 | 2.16 | 0.45 |
| 3:C:163:VAL:HG12 | 3:C:164:THR:O | 2.16 | 0.45 |
| 2:J:119:SER:HB3 | 2:J:122:ASP:HB2 | 1.99 | 0.45 |
| 3:K:18:ARG:HB2 | 3:K:18:ARG:HH11 | 1.81 | 0.45 |
| 4:L:98:ARG:HG3 | 4:L:109:ASP:OD1 | 2.17 | 0.45 |
| 1:M:344:GLN:HG2 | 1:M:349:GLU:OE2 | 2.16 | 0.45 |
| 1:M:598:GLN:H | 1:M:598:GLN:HG2 | 1.58 | 0.45 |
| 1:A:181:THR:HG23 | 1:A:195:SER:HB3 | 1.99 | 0.45 |
| 4:D:48:VAL:HG12 | 4:D:64:VAL:HG21 | 1.98 | 0.45 |
| 4:D:64:VAL:HA | 4:D:67:ARG:NH1 | 2.31 | 0.45 |
| 2:F:122:ASP:HA | 2:F:124:PHE:CE1 | 2.51 | 0.45 |
| 2:B:122:ASP:HA | 2:B:124:PHE:CE1 | 2.51 | 0.45 |
| 1:E:409:LEU:H | 1:E:409:LEU:HG | 1.50 | 0.45 |
| 1:E:471:GLU:HG2 | 1:E:472:SER:N | 2.32 | 0.45 |
| 1:E:589:GLN:CD | 1:E:589:GLN:H | 2.19 | 0.45 |
| 1:M:70:ASN:HA | 1:M:73:LYS:HE3 | 1.99 | 0.45 |
| 1:M:221:SER:HB3 | 1:M:250:PHE:HE2 | 1.81 | 0.45 |
| 1:E:549:ASN:HA | 1:E:584:MET:SD | 2.57 | 0.45 |
| 4:H:64:VAL:HA | 4:H:67:ARG:HH11 | 1.81 | 0.45 |
| 3:K:167:ASP:HB3 | 3:K:170:ASP:OD1 | 2.16 | 0.45 |
| 4:L:53:PHE:HB3 | 4:L:103:TRP:CB | 2.47 | 0.45 |
| 1:M:92:ILE:HB | 4:P:102:LYS:HE2 | 1.99 | 0.45 |
| 1:M:172:ALA:O | 1:M:178:LEU:HD12 | 2.17 | 0.45 |
| 1:M:440:GLY:N | 1:M:441:PRO:HD2 | 2.32 | 0.45 |
| 2:B:123:LEU:HD13 | 2:B:123:LEU:HA | 1.73 | 0.45 |
| 3:C:198:HIS:HB3 | 3:C:201:LEU:HG | 1.99 | 0.45 |
| 1:E:284:ASP:OD1 | 1:E:287:THR:OG1 | 2.27 | 0.45 |
| 4:H:98:ARG:HG3 | 4:H:109:ASP:OD1 | 2.17 | 0.45 |
| 3:O:50:ALA:HB3 | 3:O:53:THR:HG23 | 1.97 | 0.45 |
| 1:I:59:ALA:O | 1:I:61:VAL:N | 2.50 | 0.45 |
| 1:I:440:GLY:N | 1:I:441:PRO:HD2 | 2.31 | 0.45 |
| 1:I:518:SER:O | 1:I:522:GLU:HB2 | 2.17 | 0.45 |
| 1:A:70:ASN:HA | 1:A:73:LYS:HE3 | 1.98 | 0.45 |
| 1:A:440:GLY:N | 1:A:441:PRO:HD2 | 2.32 | 0.45 |
| 3:G:91:HIS:HB2 | 3:G:96:TRP:CZ2 | 2.51 | 0.45 |
| 1:A:622:TYR:CE1 | 1:A:657:HIS:HB2 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:108:ARG:NH2 | 3:C:140:TYR:HB2 | 2.32 | 0.44 |
| 4:D:101:TRP:HZ2 | 4:D:107:ALA:HB3 | 1.82 | 0.44 |
| 1:E:64:ASP:OD1 | 1:E:64:ASP:N | 2.50 | 0.44 |
| 1:I:242:PHE:CE1 | 1:I:288:LEU:HB3 | 2.52 | 0.44 |
| 4:P:217:LYS:HA | 4:P:217:LYS:HD3 | 1.56 | 0.44 |
| 1:E:345:SER:O | 1:E:349:GLU:HG3 | 2.17 | 0.44 |
| 2:F:48:ILE:HD12 | 2:F:89:PHE:HZ | 1.82 | 0.44 |
| 3:G:113:PRO:HD3 | 3:G:198:HIS:ND1 | 2.32 | 0.44 |
| 4:L:35:HIS:CE1 | 4:L:50:MET:HG3 | 2.52 | 0.44 |
| 1:M:25:LEU:N | 1:M:36:TYR:O | 2.42 | 0.44 |
| 1:A:549:ASN:HA | 1:A:584:MET:SD | 2.58 | 0.44 |
| 4:D:34:ILE:CG2 | 4:D:35:HIS:N | 2.80 | 0.44 |
| 4:H:217:LYS:HA | 4:H:217:LYS:HD3 | 1.49 | 0.44 |
| 1:M:252:ARG:O | 1:M:256:MET:HB2 | 2.18 | 0.44 |
| 4:H:159:THR:HB | 4:H:207:ASN:HB3 | 1.99 | 0.44 |
| 1:I:541:VAL:HA | 1:I:555:SER:HB3 | 1.99 | 0.44 |
| 2:N:48:ILE:HD12 | 2:N:89:PHE:HZ | 1.83 | 0.44 |
| 1:E:571:THR:HG23 | 1:E:573:LEU:H | 1.82 | 0.44 |
| 1:I:345:SER:O | 1:I:349:GLU:HG3 | 2.17 | 0.44 |
| 1:M:489:ASP:OD1 | 1:M:489:ASP:N | 2.38 | 0.44 |
| 3:O:195:GLU:HB2 | 3:O:206:THR:HG23 | 2.00 | 0.44 |
| 4:D:40:GLY:HA3 | 4:D:43:LYS:HE3 | 1.99 | 0.44 |
| 3:G:35:TRP:CD2 | 3:G:73:LEU:HB2 | 2.53 | 0.44 |
| 1:I:325:LEU:O | 1:I:329:LYS:N | 2.47 | 0.44 |
| 4:L:5:VAL:O | 4:L:23:VAL:N | 2.41 | 0.44 |
| 3:O:145:LYS:HB3 | 3:O:197:THR:HB | 2.00 | 0.44 |
| 1:A:21:SER:O | 1:A:40:TRP:HB2 | 2.18 | 0.44 |
| 1:A:25:LEU:N | 1:A:36:TYR:O | 2.42 | 0.44 |
| 1:A:92:ILE:O | 4:D:102:LYS:HD3 | 2.18 | 0.44 |
| 1:A:376:LEU:HD11 | 1:A:399:VAL:HG21 | 1.99 | 0.44 |
| 3:C:35:TRP:CD2 | 3:C:73:LEU:HB2 | 2.53 | 0.44 |
| 1:E:201:THR:CG2 | 1:E:225:SER:HB2 | 2.45 | 0.44 |
| 1:M:479:TYR:HA | 1:M:517:LEU:HD23 | 1.99 | 0.44 |
| 3:O:30:ARG:H | 3:O:30:ARG:HG3 | 1.50 | 0.44 |
| 4:D:12:VAL:HG11 | 4:D:18:LEU:HB2 | 2.00 | 0.44 |
| 1:E:101:GLN:HE22 | 4:H:101:TRP:HZ3 | 1.66 | 0.44 |
| 2:F:88:PHE:O | 2:F:92:ILE:HG12 | 2.17 | 0.44 |
| 3:G:167:ASP:HB3 | 3:G:170:ASP:OD1 | 2.17 | 0.44 |
| 4:H:29:PHE:HE1 | 4:H:34:ILE:HD11 | 1.82 | 0.44 |
| 1:M:101:GLN:HE22 | 4:P:101:TRP:HZ3 | 1.65 | 0.44 |
| 4:D:217:LYS:HA | 4:D:217:LYS:HD3 | 1.64 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:376:LEU:HD11 | 1:E:399:VAL:HG21 | 1.99 | 0.44 |
| 1:I:571:THR:HG23 | 1:I:573:LEU:H | 1.83 | 0.44 |
| 4:L:53:PHE:HB3 | 4:L:103:TRP:HB3 | 1.99 | 0.44 |
| 4:L:217:LYS:HA | 4:L:217:LYS:HD3 | 1.57 | 0.44 |
| 1:A:242:PHE:CE1 | 1:A:288:LEU:HB3 | 2.53 | 0.43 |
| 1:A:439:GLN:C | 1:A:441:PRO:HD2 | 2.38 | 0.43 |
| 3:G:64:GLY:HA2 | 3:G:72:THR:O | 2.17 | 0.43 |
| 1:I:279:ARG:HG3 | 1:I:280:GLU:N | 2.31 | 0.43 |
| 3:K:54:LEU:HD11 | 3:K:58:VAL:O | 2.18 | 0.43 |
| 1:M:176:LYS:HA | 1:M:176:LYS:HD3 | 1.83 | 0.43 |
| 4:D:29:PHE:HE1 | 4:D:34:ILE:HD11 | 1.83 | 0.43 |
| 4:D:32:TYR:HE1 | 4:D:101:TRP:CD1 | 2.36 | 0.43 |
| 3:G:146:VAL:HG22 | 3:G:196:VAL:HG22 | 2.00 | 0.43 |
| 1:M:409:LEU:H | 1:M:409:LEU:HG | 1.41 | 0.43 |
| 4:P:34:ILE:CG2 | 4:P:35:HIS:N | 2.81 | 0.43 |
| 1:A:122:LEU:O | 1:A:125:PRO:HD2 | 2.18 | 0.43 |
| 4:D:122:ALA:O | 4:D:123:SER:OG | 2.33 | 0.43 |
| 1:E:242:PHE:CE1 | 1:E:288:LEU:HB3 | 2.53 | 0.43 |
| 1:E:376:LEU:O | 1:E:380:THR:HG23 | 2.18 | 0.43 |
| 2:J:128:LEU:HD23 | 2:J:128:LEU:HA | 1.82 | 0.43 |
| 3:K:46:ARG:HG2 | 4:L:109:ASP:HA | 2.00 | 0.43 |
| 1:A:309:GLY:HA3 | 4:D:32:TYR:OH | 2.18 | 0.43 |
| 1:A:323:PHE:CZ | 1:A:423:ILE:HA | 2.53 | 0.43 |
| 3:C:44:PRO:HB2 | 4:D:111:PHE:CE1 | 2.53 | 0.43 |
| 1:I:271:LEU:O | 1:I:275:LYS:HD2 | 2.17 | 0.43 |
| 3:K:108:ARG:NH2 | 3:K:140:TYR:HB2 | 2.33 | 0.43 |
| 3:K:134:CYS:HB2 | 3:K:148:TRP:CH2 | 2.54 | 0.43 |
| 4:L:154:PHE:HA | 4:L:155:PRO:HA | 1.79 | 0.43 |
| 4:P:145:ALA:HB2 | 4:P:191:THR:HG22 | 2.00 | 0.43 |
| 1:E:122:LEU:O | 1:E:125:PRO:HD2 | 2.18 | 0.43 |
| 1:E:440:GLY:N | 1:E:441:PRO:HD2 | 2.33 | 0.43 |
| 1:I:122:LEU:O | 1:I:125:PRO:HD2 | 2.18 | 0.43 |
| 3:K:19:VAL:HB | 3:K:75:ILE:HG23 | 2.00 | 0.43 |
| 1:M:26:HIS:NE2 | 2:N:47:ASP:OD2 | 2.47 | 0.43 |
| 1:M:82:LEU:O | 1:M:219:ALA:HA | 2.19 | 0.43 |
| 3:O:7:THR:HG23 | 3:O:22:THR:HB | 1.99 | 0.43 |
| 4:H:39:GLN:HB2 | 4:H:45:LEU:HD23 | 2.00 | 0.43 |
| 1:I:252:ARG:O | 1:I:256:MET:HB2 | 2.18 | 0.43 |
| 3:K:124:GLN:O | 3:K:127:SER:OG | 2.34 | 0.43 |
| 4:L:48:VAL:HG12 | 4:L:64:VAL:HG21 | 2.01 | 0.43 |
| 4:P:29:PHE:CD2 | 4:P:77:ASN:HA | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:56:TRP:NE1 | 1:A:61:VAL:HG21 | 2.33 | 0.43 |
| 1:A:82:LEU:O | 1:A:219:ALA:HA | 2.19 | 0.43 |
| 4:D:10:ARG:HB2 | 4:D:18:LEU:HD21 | 2.00 | 0.43 |
| 3:G:19:VAL:HG21 | 3:G:78:LEU:HG | 2.01 | 0.43 |
| 4:H:156:GLU:HG3 | 4:H:184:TYR:CD2 | 2.53 | 0.43 |
| 3:K:21:LEU:HD22 | 3:K:102:THR:HG21 | 2.01 | 0.43 |
| 4:P:147:GLY:HA3 | 4:P:189:VAL:HG12 | 2.01 | 0.43 |
| 1:A:59:ALA:O | 1:A:61:VAL:N | 2.51 | 0.43 |
| 1:A:471:GLU:HG2 | 1:A:472:SER:N | 2.32 | 0.43 |
| 3:C:148:TRP:CG | 3:C:179:LEU:HD13 | 2.54 | 0.43 |
| 4:D:98:ARG:HG3 | 4:D:109:ASP:OD1 | 2.19 | 0.43 |
| 1:E:152:ARG:NH2 | 1:I:624:GLU:OE2 | 2.52 | 0.43 |
| 1:I:108:HIS:ND1 | 1:I:109:PRO:HD2 | 2.34 | 0.43 |
| 1:I:552:PHE:CG | 1:I:661:LEU:HD23 | 2.53 | 0.43 |
| 3:K:30:ARG:H | 3:K:30:ARG:HG3 | 1.42 | 0.43 |
| 1:M:309:GLY:HA3 | 4:P:32:TYR:OH | 2.18 | 0.43 |
| 3:O:64:GLY:HA2 | 3:O:72:THR:O | 2.18 | 0.43 |
| 4:P:31:TYR:HA | 4:P:103:TRP:HZ3 | 1.83 | 0.43 |
| 1:E:103:ASP:OD2 | 3:G:53:THR:HG22 | 2.19 | 0.43 |
| 1:E:271:LEU:O | 1:E:275:LYS:HD2 | 2.19 | 0.43 |
| 4:L:148:CYS:HB2 | 4:L:162:TRP:CZ2 | 2.54 | 0.43 |
| 1:E:323:PHE:O | 1:E:327:VAL:HG23 | 2.18 | 0.42 |
| 1:E:568:ALA:HA | 1:E:599:ILE:HD13 | 1.99 | 0.42 |
| 3:G:163:VAL:HG12 | 3:G:164:THR:O | 2.19 | 0.42 |
| 1:I:149:TYR:CE2 | 1:I:208:ARG:HA | 2.54 | 0.42 |
| 1:I:181:THR:HA | 1:I:195:SER:HA | 2.01 | 0.42 |
| 1:I:190:ASP:OD1 | 1:I:190:ASP:N | 2.52 | 0.42 |
| 1:M:149:TYR:CE2 | 1:M:208:ARG:HA | 2.55 | 0.42 |
| 1:M:482:LEU:HD13 | 1:M:546:PRO:HD3 | 2.01 | 0.42 |
| 1:A:103:ASP:OD2 | 3:C:53:THR:HG22 | 2.19 | 0.42 |
| 1:A:552:PHE:CG | 1:A:661:LEU:HD23 | 2.54 | 0.42 |
| 1:E:139:PRO:HB2 | 1:E:141:THR:HG22 | 2.01 | 0.42 |
| 3:G:121:SER:OG | 4:H:130:PHE:HB3 | 2.19 | 0.42 |
| 1:I:471:GLU:HG2 | 1:I:472:SER:N | 2.34 | 0.42 |
| 1:I:558:ARG:NH2 | 1:I:594:GLY:O | 2.52 | 0.42 |
| 3:K:115:VAL:HA | 3:K:135:LEU:O | 2.19 | 0.42 |
| 4:L:122:ALA:O | 4:L:123:SER:OG | 2.29 | 0.42 |
| 1:M:539:ASP:OD1 | 1:M:539:ASP:N | 2.53 | 0.42 |
| 4:P:48:VAL:HG12 | 4:P:64:VAL:HG21 | 2.01 | 0.42 |
| 1:A:149:TYR:CE2 | 1:A:208:ARG:HA | 2.54 | 0.42 |
| 4:D:6:GLU:HG2 | 4:D:96:CYS:SG | 2.59 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:8:GLY:HA3 | 4:H:20:LEU:HA | 2.00 | 0.42 |
| 4:H:173:THR:HG23 | 4:H:188:SER:HB2 | 2.01 | 0.42 |
| 1:I:172:ALA:O | 1:I:178:LEU:HD12 | 2.19 | 0.42 |
| 3:K:93:THR:O | 3:K:93:THR:OG1 | 2.36 | 0.42 |
| 1:M:103:ASP:OD2 | 3:O:53:THR:HG22 | 2.19 | 0.42 |
| 1:A:108:HIS:ND1 | 1:A:109:PRO:HD2 | 2.33 | 0.42 |
| 3:C:145:LYS:HB3 | 3:C:197:THR:HB | 2.01 | 0.42 |
| 1:I:430:ARG:HA | 1:I:433:ARG:HG3 | 2.00 | 0.42 |
| 1:I:479:TYR:HA | 1:I:517:LEU:HD23 | 2.00 | 0.42 |
| 4:L:152:ASP:HA | 4:L:183:LEU:HB3 | 2.01 | 0.42 |
| 1:M:125:PRO:HA | 1:M:128:LYS:HE2 | 2.01 | 0.42 |
| 3:G:108:ARG:NH2 | 3:G:140:TYR:HB2 | 2.34 | 0.42 |
| 3:C:19:VAL:HG21 | 3:C:78:LEU:HG | 2.02 | 0.42 |
| 4:H:35:HIS:CE1 | 4:H:50:MET:HG3 | 2.55 | 0.42 |
| 1:I:62:THR:HB | 2:J:33:GLN:HA | 2.01 | 0.42 |
| 2:J:122:ASP:HA | 2:J:124:PHE:CE1 | 2.54 | 0.42 |
| 3:K:107:LYS:HG3 | 3:K:108:ARG:N | 2.34 | 0.42 |
| 4:L:100:GLY:HA2 | 4:L:105:GLY:O | 2.19 | 0.42 |
| 4:L:103:TRP:CD1 | 4:L:104:PRO:HD3 | 2.55 | 0.42 |
| 1:M:108:HIS:ND1 | 1:M:109:PRO:HD2 | 2.34 | 0.42 |
| 1:M:148:PHE:CZ | 1:M:197:ILE:CD1 | 3.03 | 0.42 |
| 1:M:329:LYS:NZ | 1:M:340:VAL:HB | 2.35 | 0.42 |
| 1:A:69:LEU:HD23 | 1:I:79:SER:HA | 2.02 | 0.42 |
| 2:F:123:LEU:HD13 | 2:F:123:LEU:HA | 1.71 | 0.42 |
| 4:H:32:TYR:HE1 | 4:H:101:TRP:CD1 | 2.38 | 0.42 |
| 1:I:572:TYR:CG | 1:I:572:TYR:O | 2.72 | 0.42 |
| 3:K:150:VAL:HB | 3:K:155:GLN:HE21 | 1.84 | 0.42 |
| 1:M:214:PRO:O | 2:F:125:GLY:HA3 | 2.20 | 0.42 |
| 4:P:53:PHE:HB3 | 4:P:103:TRP:CB | 2.48 | 0.42 |
| 3:C:115:VAL:HA | 3:C:135:LEU:O | 2.19 | 0.42 |
| 1:E:59:ALA:O | 1:E:61:VAL:N | 2.53 | 0.42 |
| 1:I:361:MET:O | 1:I:395:GLY:HA2 | 2.20 | 0.42 |
| 1:M:331:ILE:HA | 1:M:334:ILE:HG12 | 2.01 | 0.42 |
| 4:P:159:THR:HB | 4:P:207:ASN:HB3 | 2.01 | 0.42 |
| 3:G:115:VAL:HA | 3:G:135:LEU:O | 2.19 | 0.42 |
| 3:G:136:LEU:HB2 | 3:G:175:LEU:HB3 | 2.02 | 0.42 |
| 4:H:100:GLY:HA2 | 4:H:105:GLY:O | 2.20 | 0.42 |
| 4:H:152:ASP:HA | 4:H:183:LEU:HB3 | 2.01 | 0.42 |
| 1:I:464:ARG:HB2 | 1:I:496:PRO:HG3 | 2.01 | 0.42 |
| 1:M:60:ASN:CB | 1:M:63:GLU:HB2 | 2.47 | 0.42 |
| 3:C:142:ARG:HD2 | 3:C:163:VAL:HG11 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:439:GLN:C | 1:I:441:PRO:HD2 | 2.40 | 0.42 |
| 3:K:78:LEU:HD23 | 3:K:78:LEU:HA | 1.93 | 0.42 |
| 1:M:59:ALA:O | 1:M:61:VAL:N | 2.53 | 0.41 |
| 1:M:181:THR:HA | 1:M:195:SER:HA | 2.01 | 0.41 |
| 1:M:614:PHE:O | 1:M:634:ILE:HB | 2.20 | 0.41 |
| 4:P:53:PHE:HB3 | 4:P:103:TRP:HB3 | 2.01 | 0.41 |
| 4:P:64:VAL:HA | 4:P:67:ARG:NH1 | 2.33 | 0.41 |
| 1:A:181:THR:HA | 1:A:195:SER:HA | 2.00 | 0.41 |
| 1:A:393:ILE:HG12 | 1:A:431:GLU:HG3 | 2.01 | 0.41 |
| 1:A:614:PHE:O | 1:A:634:ILE:HB | 2.20 | 0.41 |
| 3:G:6:GLN:HG3 | 3:G:99:GLY:HA3 | 2.02 | 0.41 |
| 4:H:53:PHE:HB3 | 4:H:103:TRP:CB | 2.50 | 0.41 |
| 1:I:453:LEU:HD23 | 1:I:453:LEU:HA | 1.87 | 0.41 |
| 1:I:459:ILE:O | 1:I:463:LEU:HG | 2.20 | 0.41 |
| 1:E:323:PHE:CZ | 1:E:423:ILE:HA | 2.55 | 0.41 |
| 1:E:552:PHE:CE2 | 1:E:581:PRO:HB3 | 2.55 | 0.41 |
| 2:F:47:ASP:HB2 | 2:F:65:ASN:OD1 | 2.20 | 0.41 |
| 3:G:108:ARG:HD3 | 3:G:171:SER:HB2 | 2.02 | 0.41 |
| 3:G:186:TYR:HA | 3:G:192:TYR:OH | 2.20 | 0.41 |
| 1:I:329:LYS:NZ | 1:I:340:VAL:HB | 2.35 | 0.41 |
| 4:L:31:TYR:HA | 4:L:103:TRP:HZ3 | 1.83 | 0.41 |
| 1:M:583:ILE:HD13 | 1:M:583:ILE:HA | 1.90 | 0.41 |
| 4:P:154:PHE:HA | 4:P:155:PRO:HA | 1.81 | 0.41 |
| 1:A:198:PHE:HB2 | 1:A:226:LEU:HD13 | 2.01 | 0.41 |
| 1:E:176:LYS:HA | 1:E:176:LYS:HD3 | 1.83 | 0.41 |
| 1:M:179:MET:HA | 1:M:196:LEU:O | 2.20 | 0.41 |
| 1:A:491:LEU:HD12 | 1:A:510:VAL:HG13 | 2.01 | 0.41 |
| 3:K:46:ARG:CZ | 3:K:55:GLU:HB3 | 2.51 | 0.41 |
| 1:M:169:TYR:OH | 1:M:292:PHE:HA | 2.21 | 0.41 |
| 1:M:275:LYS:HE3 | 1:M:275:LYS:N | 2.35 | 0.41 |
| 3:C:6:GLN:HG3 | 3:C:99:GLY:HA3 | 2.02 | 0.41 |
| 3:C:136:LEU:HB2 | 3:C:175:LEU:HB3 | 2.02 | 0.41 |
| 1:I:549:ASN:HA | 1:I:584:MET:SD | 2.59 | 0.41 |
| 1:M:50:LEU:HG | 1:M:52:PRO:HD3 | 2.01 | 0.41 |
| 1:M:464:ARG:NH2 | 1:M:496:PRO:HB3 | 2.35 | 0.41 |
| 1:M:541:VAL:HA | 1:M:555:SER:CB | 2.50 | 0.41 |
| 2:N:119:SER:HB3 | 2:N:122:ASP:HB2 | 2.01 | 0.41 |
| 4:P:31:TYR:HA | 4:P:103:TRP:CZ3 | 2.54 | 0.41 |
| 4:P:32:TYR:HE1 | 4:P:101:TRP:CD1 | 2.34 | 0.41 |
| 1:A:24:LYS:HA | 1:A:37:THR:HA | 2.02 | 0.41 |
| 3:G:48:ILE:HD12 | 3:G:73:LEU:HD12 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:209:GLY:O | 2:N:115:TYR:OH | 2.34 | 0.41 |
| 1:M:361:MET:O | 1:M:395:GLY:HA2 | 2.20 | 0.41 |
| 1:M:393:ILE:HG12 | 1:M:431:GLU:HG3 | 2.02 | 0.41 |
| 1:M:552:PHE:CG | 1:M:661:LEU:HD23 | 2.55 | 0.41 |
| 4:P:34:ILE:HG21 | 4:P:79:LEU:CD2 | 2.50 | 0.41 |
| 4:H:154:PHE:HA | 4:H:155:PRO:HA | 1.82 | 0.41 |
| 4:H:211:SER:OG | 4:H:213:THR:OG1 | 2.29 | 0.41 |
| 1:I:409:LEU:H | 1:I:409:LEU:HG | 1.43 | 0.41 |
| 4:L:29:PHE:CD2 | 4:L:77:ASN:HA | 2.56 | 0.41 |
| 4:L:30:SER:HA | 4:L:72:ARG:NH2 | 2.35 | 0.41 |
| 1:M:451:THR:HA | 1:M:481:SER:HB2 | 2.03 | 0.41 |
| 1:A:390:SER:OG | 1:A:438:THR:HB | 2.20 | 0.41 |
| 1:E:156:SER:O | 1:E:173:MET:HG2 | 2.21 | 0.41 |
| 1:E:329:LYS:NZ | 1:E:340:VAL:HB | 2.36 | 0.41 |
| 1:E:459:ILE:O | 1:E:463:LEU:HG | 2.21 | 0.41 |
| 3:K:44:PRO:HB2 | 4:L:111:PHE:CE1 | 2.55 | 0.41 |
| 1:M:491:LEU:HD12 | 1:M:510:VAL:HG13 | 2.03 | 0.41 |
| 3:C:121:SER:OG | 4:D:130:PHE:HB3 | 2.20 | 0.41 |
| 3:C:186:TYR:HA | 3:C:192:TYR:OH | 2.20 | 0.41 |
| 4:D:29:PHE:CE1 | 4:D:34:ILE:HD11 | 2.56 | 0.41 |
| 1:E:50:LEU:HD21 | 2:F:92:ILE:HG23 | 2.03 | 0.41 |
| 1:E:78:THR:HB | 1:E:81:THR:HB | 2.03 | 0.41 |
| 3:G:35:TRP:CE2 | 3:G:73:LEU:HB2 | 2.56 | 0.41 |
| 1:I:36:TYR:HD2 | 2:J:103:HIS:CE1 | 2.39 | 0.41 |
| 1:I:67:SER:HA | 1:I:70:ASN:HB2 | 2.01 | 0.41 |
| 1:I:149:TYR:CD2 | 1:I:208:ARG:HA | 2.56 | 0.41 |
| 1:I:482:LEU:HD13 | 1:I:546:PRO:HD3 | 2.03 | 0.41 |
| 2:J:124:PHE:C | 2:J:126:ALA:H | 2.25 | 0.41 |
| 1:A:612:CYS:O | 1:A:614:PHE:N | 2.54 | 0.41 |
| 1:E:21:SER:O | 1:E:40:TRP:HB2 | 2.20 | 0.41 |
| 1:E:149:TYR:CE2 | 1:E:208:ARG:HA | 2.56 | 0.41 |
| 1:I:59:ALA:HB1 | 2:J:84:ASN:HB3 | 2.03 | 0.41 |
| 3:K:121:SER:OG | 4:L:130:PHE:HB3 | 2.20 | 0.41 |
| 1:M:139:PRO:HB2 | 1:M:141:THR:H | 1.87 | 0.40 |
| 1:M:156:SER:HB2 | 1:M:342:GLY:O | 2.21 | 0.40 |
| 2:N:128:LEU:HD23 | 2:N:128:LEU:HA | 1.80 | 0.40 |
| 3:O:197:THR:HG23 | 3:O:204:PRO:HG3 | 2.02 | 0.40 |
| 4:P:27:PHE:CE2 | 4:P:98:ARG:HD2 | 2.55 | 0.40 |
| 4:P:35:HIS:CD2 | 4:P:99:GLY:HA3 | 2.55 | 0.40 |
| 1:A:179:MET:HA | 1:A:196:LEU:O | 2.21 | 0.40 |
| 1:A:275:LYS:HE3 | 1:A:275:LYS:N | 2.35 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:29:PHE:CE1 | 4:H:34:ILE:HD11 | 2.56 | 0.40 |
| 1:I:231:THR:HB | 1:I:234:HIS:H | 1.86 | 0.40 |
| 1:I:249:MET:SD | 1:I:289:THR:HG23 | 2.61 | 0.40 |
| 1:M:311:GLY:HA3 | 4:P:101:TRP:HB2 | 2.02 | 0.40 |
| 1:M:390:SER:OG | 1:M:438:THR:HB | 2.21 | 0.40 |
| 3:O:108:ARG:NH2 | 3:O:140:TYR:HB2 | 2.35 | 0.40 |
| 3:C:150:VAL:HG22 | 3:C:192:TYR:CD1 | 2.56 | 0.40 |
| 1:E:482:LEU:HD13 | 1:E:546:PRO:HD3 | 2.02 | 0.40 |
| 2:F:128:LEU:HD23 | 2:F:128:LEU:HA | 1.82 | 0.40 |
| 1:I:543:MET:HE3 | 1:I:543:MET:HB2 | 1.91 | 0.40 |
| 1:I:632:THR:HG21 | 1:I:643:ILE:HD11 | 2.03 | 0.40 |
| 1:A:252:ARG:O | 1:A:256:MET:HB2 | 2.21 | 0.40 |
| 4:D:154:PHE:HA | 4:D:155:PRO:HA | 1.79 | 0.40 |
| 4:L:148:CYS:N | 4:L:188:SER:O | 2.53 | 0.40 |
| 1:M:196:LEU:HD12 | 1:M:196:LEU:HA | 1.84 | 0.40 |
| 1:M:323:PHE:CZ | 1:M:423:ILE:HA | 2.57 | 0.40 |
| 1:A:149:TYR:CD2 | 1:A:208:ARG:HA | 2.57 | 0.40 |
| 1:A:169:TYR:OH | 1:A:292:PHE:HA | 2.22 | 0.40 |
| 3:C:7:THR:HG23 | 3:C:22:THR:HB | 2.03 | 0.40 |
| 1:E:252:ARG:O | 1:E:256:MET:HB2 | 2.21 | 0.40 |
| 1:E:439:GLN:C | 1:E:441:PRO:HD2 | 2.42 | 0.40 |
| 4:H:150:VAL:HG11 | 4:H:158:VAL:HG11 | 2.04 | 0.40 |
| 4:L:31:TYR:HA | 4:L:103:TRP:CZ3 | 2.56 | 0.40 |
| 3:O:148:TRP:CG | 3:O:179:LEU:HD13 | 2.57 | 0.40 |
| 1:A:73:LYS:HZ1 | 1:I:79:SER:HB3 | 1.85 | 0.40 |
| 1:A:376:LEU:O | 1:A:380:THR:HG23 | 2.21 | 0.40 |
| 1:A:598:GLN:H | 1:A:598:GLN:HG2 | 1.64 | 0.40 |
| 2:B:125:GLY:HA3 | 1:I:214:PRO:O | 2.21 | 0.40 |
| 3:C:107:LYS:HG3 | 3:C:108:ARG:N | 2.36 | 0.40 |
| 3:G:50:ALA:C | 3:G:52:SER:H | 2.24 | 0.40 |
| 3:G:96:TRP:CZ3 | 4:H:35:HIS:CE1 | 3.10 | 0.40 |
| 1:I:79:SER:O | 1:I:81:THR:HG22 | 2.22 | 0.40 |
| 3:K:140:TYR:CD1 | 3:K:141:PRO:HA | 2.57 | 0.40 |
| 4:L:101:TRP:HZ2 | 4:L:107:ALA:HB3 | 1.87 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | A | 653/665 (98%) | 609 (93%) | 44 (7%) | 0 | 100 | 100 |
| 1 | E | 653/665 (98%) | 613 (94%) | 40 (6%) | 0 | 100 | 100 |
| 1 | I | 653/665 (98%) | 606 (93%) | 47 (7%) | 0 | 100 | 100 |
| 1 | M | 653/665 (98%) | 606 (93%) | 47 (7%) | 0 | 100 | 100 |
| 2 | B | 88/112 (79%) | 79 (90%) | 8 (9%) | 1 (1%) | 14 | 52 |
| 2 | F | 88/112 (79%) | 80 (91%) | 6 (7%) | 2 (2%) | 6 | 37 |
| 2 | J | 88/112 (79%) | 80 (91%) | 7 (8%) | 1 (1%) | 14 | 52 |
| 2 | N | 88/112 (79%) | 80 (91%) | 7 (8%) | 1 (1%) | 14 | 52 |
| 3 | C | 211/233 (91%) | 200 (95%) | 11 (5%) | 0 | 100 | 100 |
| 3 | G | 211/233 (91%) | 198 (94%) | 13 (6%) | 0 | 100 | 100 |
| 3 | K | 211/233 (91%) | 201 (95%) | 10 (5%) | 0 | 100 | 100 |
| 3 | O | 211/233 (91%) | 199 (94%) | 12 (6%) | 0 | 100 | 100 |
| 4 | D | 210/470 (45%) | 197 (94%) | 13 (6%) | 0 | 100 | 100 |
| 4 | H | 210/470 (45%) | 197 (94%) | 13 (6%) | 0 | 100 | 100 |
| 4 | L | 210/470 (45%) | 196 (93%) | 14 (7%) | 0 | 100 | 100 |
| 4 | P | 210/470 (45%) | 198 (94%) | 12 (6%) | 0 | 100 | 100 |
| All | All | 4648/5920 (78%) | 4339 (93%) | 304 (6%) | 5 (0%) | 51 | 85 |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | N | 124 | PHE |
| 2 | B | 124 | PHE |
| 2 | F | 124 | PHE |
| 2 | J | 124 | PHE |
| 2 | F | 125 | GLY |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1 | A | 561/570 (98%) | 505 (90%) | 56 (10%) | 7 | 28 |
| 1 | E | 561/570 (98%) | 507 (90%) | 54 (10%) | 8 | 30 |
| 1 | I | 561/570 (98%) | 504 (90%) | 57 (10%) | 7 | 28 |
| 1 | M | 561/570 (98%) | 507 (90%) | 54 (10%) | 8 | 30 |
| 2 | B | 83/99 (84%) | 74 (89%) | 9 (11%) | 6 | 26 |
| 2 | F | 83/99 (84%) | 74 (89%) | 9 (11%) | 6 | 26 |
| 2 | J | 83/99 (84%) | 75 (90%) | 8 (10%) | 8 | 30 |
| 2 | N | 83/99 (84%) | 74 (89%) | 9 (11%) | 6 | 26 |
| 3 | C | 186/202 (92%) | 161 (87%) | 25 (13%) | 4 | 20 |
| 3 | G | 186/202 (92%) | 164 (88%) | 22 (12%) | 5 | 23 |
| 3 | K | 186/202 (92%) | 162 (87%) | 24 (13%) | 4 | 21 |
| 3 | O | 186/202 (92%) | 162 (87%) | 24 (13%) | 4 | 21 |
| 4 | D | 180/416 (43%) | 159 (88%) | 21 (12%) | 5 | 23 |
| 4 | H | 180/416 (43%) | 158 (88%) | 22 (12%) | 5 | 23 |
| 4 | L | 180/416 (43%) | 158 (88%) | 22 (12%) | 5 | 23 |
| 4 | P | 180/416 (43%) | 155 (86%) | 25 (14%) | 3 | 20 |
| All | All | 4040/5148 (78%) | 3599 (89%) | 441 (11%) | 6 | 26 |

All (441) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 22 | GLU |
| 1 | M | 26 | HIS |
| 1 | M | 27 | LEU |
| 1 | M | 38 | ILE |
| 1 | M | 42 | GLU |
| 1 | M | 43 | LEU |
| 1 | M | 65 | LEU |
| 1 | M | 70 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 81 | THR |
| 1 | M | 84 | ILE |
| 1 | M | 95 | VAL |
| 1 | M | 153 | CYS |
| 1 | M | 163 | ASN |
| 1 | M | 194 | LEU |
| 1 | M | 196 | LEU |
| 1 | M | 213 | TYR |
| 1 | M | 221 | SER |
| 1 | M | 231 | THR |
| 1 | M | 269 | LEU |
| 1 | M | 274 | MET |
| 1 | M | 275 | LYS |
| 1 | M | 279 | ARG |
| 1 | M | 300 | LYS |
| 1 | M | 335 | CYS |
| 1 | M | 341 | LYS |
| 1 | M | 344 | GLN |
| 1 | M | 355 | LEU |
| 1 | M | 359 | VAL |
| 1 | M | 370 | GLU |
| 1 | M | 385 | LYS |
| 1 | M | 389 | TYR |
| 1 | M | 409 | LEU |
| 1 | M | 442 | ASN |
| 1 | M | 445 | LEU |
| 1 | M | 457 | LEU |
| 1 | M | 471 | GLU |
| 1 | M | 489 | ASP |
| 1 | M | 492 | LEU |
| 1 | M | 503 | GLN |
| 1 | M | 508 | ASN |
| 1 | M | 517 | LEU |
| 1 | M | 519 | LEU |
| 1 | M | 521 | ARG |
| 1 | M | 525 | ASP |
| 1 | M | 529 | LEU |
| 1 | M | 532 | TYR |
| 1 | M | 570 | THR |
| 1 | M | 572 | TYR |
| 1 | M | 573 | LEU |
| 1 | M | 576 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 601 | LYS |
| 1 | M | 606 | THR |
| 1 | M | 615 | CYS |
| 1 | M | 632 | THR |
| 2 | N | 40 | LEU |
| 2 | N | 53 | ASN |
| 2 | N | 77 | SER |
| 2 | N | 78 | ARG |
| 2 | N | 98 | SER |
| 2 | N | 100 | LEU |
| 2 | N | 114 | LEU |
| 2 | N | 123 | LEU |
| 2 | N | 127 | ASN |
| 3 | O | 1 | ASP |
| 3 | O | 5 | THR |
| 3 | O | 11 | LEU |
| 3 | O | 15 | VAL |
| 3 | O | 30 | ARG |
| 3 | O | 46 | ARG |
| 3 | O | 49 | TYR |
| 3 | O | 75 | ILE |
| 3 | O | 78 | LEU |
| 3 | O | 83 | PHE |
| 3 | O | 85 | THR |
| 3 | O | 100 | GLN |
| 3 | O | 103 | LYS |
| 3 | O | 107 | LYS |
| 3 | O | 121 | SER |
| 3 | O | 129 | THR |
| 3 | O | 133 | VAL |
| 3 | O | 142 | ARG |
| 3 | O | 143 | GLU |
| 3 | O | 147 | GLN |
| 3 | O | 154 | LEU |
| 3 | O | 176 | SER |
| 3 | O | 187 | GLU |
| 3 | O | 206 | THR |
| 4 | P | 3 | GLN |
| 4 | P | 6 | GLU |
| 4 | P | 13 | GLN |
| 4 | P | 25 | SER |
| 4 | P | 28 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | P | 48 | VAL |
| 4 | P | 53 | PHE |
| 4 | P | 54 | ASP |
| 4 | P | 60 | CYS |
| 4 | P | 98 | ARG |
| 4 | P | 101 | TRP |
| 4 | P | 102 | LYS |
| 4 | P | 103 | TRP |
| 4 | P | 108 | PHE |
| 4 | P | 109 | ASP |
| 4 | P | 115 | THR |
| 4 | P | 116 | VAL |
| 4 | P | 118 | THR |
| 4 | P | 128 | SER |
| 4 | P | 148 | CYS |
| 4 | P | 187 | SER |
| 4 | P | 189 | VAL |
| 4 | P | 194 | SER |
| 4 | P | 204 | CYS |
| 4 | P | 212 | ASN |
| 1 | A | 26 | HIS |
| 1 | A | 27 | LEU |
| 1 | A | 30 | GLU |
| 1 | A | 38 | ILE |
| 1 | A | 42 | GLU |
| 1 | A | 43 | LEU |
| 1 | A | 65 | LEU |
| 1 | A | 70 | ASN |
| 1 | A | 81 | THR |
| 1 | A | 84 | ILE |
| 1 | A | 163 | ASN |
| 1 | A | 170 | THR |
| 1 | A | 188 | LYS |
| 1 | A | 194 | LEU |
| 1 | A | 196 | LEU |
| 1 | A | 206 | ASP |
| 1 | A | 213 | TYR |
| 1 | A | 218 | SER |
| 1 | A | 231 | THR |
| 1 | A | 269 | LEU |
| 1 | A | 274 | MET |
| 1 | A | 275 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 300 | LYS |
| 1 | A | 330 | ASP |
| 1 | A | 335 | CYS |
| 1 | A | 341 | LYS |
| 1 | A | 344 | GLN |
| 1 | A | 355 | LEU |
| 1 | A | 359 | VAL |
| 1 | A | 370 | GLU |
| 1 | A | 385 | LYS |
| 1 | A | 389 | TYR |
| 1 | A | 409 | LEU |
| 1 | A | 442 | ASN |
| 1 | A | 445 | LEU |
| 1 | A | 457 | LEU |
| 1 | A | 471 | GLU |
| 1 | A | 489 | ASP |
| 1 | A | 490 | LYS |
| 1 | A | 492 | LEU |
| 1 | A | 503 | GLN |
| 1 | A | 508 | ASN |
| 1 | A | 517 | LEU |
| 1 | A | 519 | LEU |
| 1 | A | 521 | ARG |
| 1 | A | 525 | ASP |
| 1 | A | 529 | LEU |
| 1 | A | 532 | TYR |
| 1 | A | 570 | THR |
| 1 | A | 572 | TYR |
| 1 | A | 573 | LEU |
| 1 | A | 576 | SER |
| 1 | A | 601 | LYS |
| 1 | A | 606 | THR |
| 1 | A | 615 | CYS |
| 1 | A | 632 | THR |
| 2 | B | 40 | LEU |
| 2 | B | 53 | ASN |
| 2 | B | 77 | SER |
| 2 | B | 78 | ARG |
| 2 | B | 98 | SER |
| 2 | B | 100 | LEU |
| 2 | B | 114 | LEU |
| 2 | B | 123 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 127 | ASN |
| 3 | C | 1 | ASP |
| 3 | C | 5 | THR |
| 3 | C | 11 | LEU |
| 3 | C | 15 | VAL |
| 3 | C | 18 | ARG |
| 3 | C | 30 | ARG |
| 3 | C | 46 | ARG |
| 3 | C | 49 | TYR |
| 3 | C | 75 | ILE |
| 3 | C | 78 | LEU |
| 3 | C | 83 | PHE |
| 3 | C | 85 | THR |
| 3 | C | 100 | GLN |
| 3 | C | 103 | LYS |
| 3 | C | 107 | LYS |
| 3 | C | 121 | SER |
| 3 | C | 129 | THR |
| 3 | C | 133 | VAL |
| 3 | C | 142 | ARG |
| 3 | C | 143 | GLU |
| 3 | C | 147 | GLN |
| 3 | C | 154 | LEU |
| 3 | C | 176 | SER |
| 3 | C | 187 | GLU |
| 3 | C | 206 | THR |
| 4 | D | 3 | GLN |
| 4 | D | 6 | GLU |
| 4 | D | 13 | GLN |
| 4 | D | 25 | SER |
| 4 | D | 28 | THR |
| 4 | D | 48 | VAL |
| 4 | D | 53 | PHE |
| 4 | D | 54 | ASP |
| 4 | D | 60 | CYS |
| 4 | D | 98 | ARG |
| 4 | D | 101 | TRP |
| 4 | D | 102 | LYS |
| 4 | D | 103 | TRP |
| 4 | D | 108 | PHE |
| 4 | D | 109 | ASP |
| 4 | D | 115 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 116 | VAL |
| 4 | D | 118 | THR |
| 4 | D | 148 | CYS |
| 4 | D | 194 | SER |
| 4 | D | 212 | ASN |
| 1 | E | 22 | GLU |
| 1 | E | 26 | HIS |
| 1 | E | 27 | LEU |
| 1 | E | 38 | ILE |
| 1 | E | 41 | THR |
| 1 | E | 42 | GLU |
| 1 | E | 43 | LEU |
| 1 | E | 57 | ARG |
| 1 | E | 70 | ASN |
| 1 | E | 81 | THR |
| 1 | E | 95 | VAL |
| 1 | E | 115 | LEU |
| 1 | E | 153 | CYS |
| 1 | E | 163 | ASN |
| 1 | E | 194 | LEU |
| 1 | E | 196 | LEU |
| 1 | E | 206 | ASP |
| 1 | E | 213 | TYR |
| 1 | E | 218 | SER |
| 1 | E | 221 | SER |
| 1 | E | 225 | SER |
| 1 | E | 269 | LEU |
| 1 | E | 274 | MET |
| 1 | E | 275 | LYS |
| 1 | E | 300 | LYS |
| 1 | E | 335 | CYS |
| 1 | E | 341 | LYS |
| 1 | E | 344 | GLN |
| 1 | E | 355 | LEU |
| 1 | E | 359 | VAL |
| 1 | E | 370 | GLU |
| 1 | E | 385 | LYS |
| 1 | E | 389 | TYR |
| 1 | E | 409 | LEU |
| 1 | E | 442 | ASN |
| 1 | E | 445 | LEU |
| 1 | E | 457 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 471 | GLU |
| 1 | E | 489 | ASP |
| 1 | E | 492 | LEU |
| 1 | E | 503 | GLN |
| 1 | E | 508 | ASN |
| 1 | E | 517 | LEU |
| 1 | E | 519 | LEU |
| 1 | E | 521 | ARG |
| 1 | E | 525 | ASP |
| 1 | E | 532 | TYR |
| 1 | E | 558 | ARG |
| 1 | E | 569 | SER |
| 1 | E | 570 | THR |
| 1 | E | 572 | TYR |
| 1 | E | 573 | LEU |
| 1 | E | 601 | LYS |
| 1 | E | 615 | CYS |
| 2 | F | 40 | LEU |
| 2 | F | 53 | ASN |
| 2 | F | 78 | ARG |
| 2 | F | 98 | SER |
| 2 | F | 100 | LEU |
| 2 | F | 101 | THR |
| 2 | F | 114 | LEU |
| 2 | F | 123 | LEU |
| 2 | F | 127 | ASN |
| 3 | G | 5 | THR |
| 3 | G | 11 | LEU |
| 3 | G | 15 | VAL |
| 3 | G | 30 | ARG |
| 3 | G | 46 | ARG |
| 3 | G | 49 | TYR |
| 3 | G | 73 | LEU |
| 3 | G | 75 | ILE |
| 3 | G | 78 | LEU |
| 3 | G | 83 | PHE |
| 3 | G | 85 | THR |
| 3 | G | 100 | GLN |
| 3 | G | 103 | LYS |
| 3 | G | 107 | LYS |
| 3 | G | 121 | SER |
| 3 | G | 129 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | G | 133 | VAL |
| 3 | G | 143 | GLU |
| 3 | G | 147 | GLN |
| 3 | G | 154 | LEU |
| 3 | G | 176 | SER |
| 3 | G | 187 | GLU |
| 4 | H | 3 | GLN |
| 4 | H | 6 | GLU |
| 4 | H | 10 | ARG |
| 4 | H | 13 | GLN |
| 4 | H | 21 | SER |
| 4 | H | 25 | SER |
| 4 | H | 28 | THR |
| 4 | H | 48 | VAL |
| 4 | H | 49 | THR |
| 4 | H | 54 | ASP |
| 4 | H | 60 | CYS |
| 4 | H | 98 | ARG |
| 4 | H | 101 | TRP |
| 4 | H | 102 | LYS |
| 4 | H | 103 | TRP |
| 4 | H | 108 | PHE |
| 4 | H | 109 | ASP |
| 4 | H | 115 | THR |
| 4 | H | 148 | CYS |
| 4 | H | 187 | SER |
| 4 | H | 194 | SER |
| 4 | H | 204 | CYS |
| 1 | I | 22 | GLU |
| 1 | I | 26 | HIS |
| 1 | I | 27 | LEU |
| 1 | I | 38 | ILE |
| 1 | I | 41 | THR |
| 1 | I | 42 | GLU |
| 1 | I | 43 | LEU |
| 1 | I | 70 | ASN |
| 1 | I | 79 | SER |
| 1 | I | 81 | THR |
| 1 | I | 84 | ILE |
| 1 | I | 95 | VAL |
| 1 | I | 153 | CYS |
| 1 | I | 163 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 194 | LEU |
| 1 | I | 196 | LEU |
| 1 | I | 213 | TYR |
| 1 | I | 218 | SER |
| 1 | I | 221 | SER |
| 1 | I | 231 | THR |
| 1 | I | 269 | LEU |
| 1 | I | 274 | MET |
| 1 | I | 275 | LYS |
| 1 | I | 278 | CYS |
| 1 | I | 279 | ARG |
| 1 | I | 300 | LYS |
| 1 | I | 341 | LYS |
| 1 | I | 344 | GLN |
| 1 | I | 355 | LEU |
| 1 | I | 359 | VAL |
| 1 | I | 370 | GLU |
| 1 | I | 385 | LYS |
| 1 | I | 389 | TYR |
| 1 | I | 409 | LEU |
| 1 | I | 442 | ASN |
| 1 | I | 445 | LEU |
| 1 | I | 457 | LEU |
| 1 | I | 471 | GLU |
| 1 | I | 489 | ASP |
| 1 | I | 490 | LYS |
| 1 | I | 492 | LEU |
| 1 | I | 503 | GLN |
| 1 | I | 508 | ASN |
| 1 | I | 517 | LEU |
| 1 | I | 519 | LEU |
| 1 | I | 521 | ARG |
| 1 | I | 525 | ASP |
| 1 | I | 529 | LEU |
| 1 | I | 532 | TYR |
| 1 | I | 569 | SER |
| 1 | I | 570 | THR |
| 1 | I | 572 | TYR |
| 1 | I | 573 | LEU |
| 1 | I | 574 | SER |
| 1 | I | 576 | SER |
| 1 | I | 601 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 606 | THR |
| 2 | J | 40 | LEU |
| 2 | J | 53 | ASN |
| 2 | J | 77 | SER |
| 2 | J | 78 | ARG |
| 2 | J | 98 | SER |
| 2 | J | 100 | LEU |
| 2 | J | 123 | LEU |
| 2 | J | 127 | ASN |
| 3 | K | 1 | ASP |
| 3 | K | 5 | THR |
| 3 | K | 11 | LEU |
| 3 | K | 15 | VAL |
| 3 | K | 30 | ARG |
| 3 | K | 46 | ARG |
| 3 | K | 49 | TYR |
| 3 | K | 73 | LEU |
| 3 | K | 75 | ILE |
| 3 | K | 78 | LEU |
| 3 | K | 83 | PHE |
| 3 | K | 85 | THR |
| 3 | K | 100 | GLN |
| 3 | K | 103 | LYS |
| 3 | K | 107 | LYS |
| 3 | K | 121 | SER |
| 3 | K | 129 | THR |
| 3 | K | 133 | VAL |
| 3 | K | 142 | ARG |
| 3 | K | 143 | GLU |
| 3 | K | 147 | GLN |
| 3 | K | 176 | SER |
| 3 | K | 187 | GLU |
| 3 | K | 199 | GLN |
| 4 | L | 3 | GLN |
| 4 | L | 6 | GLU |
| 4 | L | 10 | ARG |
| 4 | L | 13 | GLN |
| 4 | L | 21 | SER |
| 4 | L | 25 | SER |
| 4 | L | 28 | THR |
| 4 | L | 48 | VAL |
| 4 | L | 53 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | L | 54 | ASP |
| 4 | L | 60 | CYS |
| 4 | L | 98 | ARG |
| 4 | L | 101 | TRP |
| 4 | L | 102 | LYS |
| 4 | L | 103 | TRP |
| 4 | L | 108 | PHE |
| 4 | L | 109 | ASP |
| 4 | L | 115 | THR |
| 4 | L | 118 | THR |
| 4 | L | 148 | CYS |
| 4 | L | 187 | SER |
| 4 | L | 194 | SER |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | P | 35 | HIS |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1 | A | 655/665 (98%) | -0.17 | 10 (1%) 73 64 | 59, 142, 223, 269 | 0 |
| 1 | E | 655/665 (98%) | 0.18 | 38 (5%) 23 19 | 64, 184, 281, 343 | 0 |
| 1 | I | 655/665 (98%) | -0.16 | 11 (1%) 70 61 | 58, 140, 220, 266 | 0 |
| 1 | M | 655/665 (98%) | -0.11 | 10 (1%) 73 64 | 67, 155, 224, 267 | 0 |
| 2 | B | 94/112 (83%) | 0.30 | 8 (8%) 10 10 | 96, 169, 218, 269 | 0 |
| 2 | F | 94/112 (83%) | 0.23 | 5 (5%) 26 23 | 105, 177, 229, 279 | 0 |
| 2 | J | 94/112 (83%) | 0.12 | 3 (3%) 47 37 | 94, 170, 215, 266 | 0 |
| 2 | N | 94/112 (83%) | 0.48 | 11 (11%) 4 5 | 104, 186, 232, 277 | 0 |
| 3 | C | 213/233 (91%) | -0.14 | 0 100 100 | 72, 118, 162, 211 | 0 |
| 3 | G | 213/233 (91%) | -0.03 | 1 (0%) 91 86 | 86, 122, 167, 219 | 0 |
| 3 | K | 213/233 (91%) | -0.16 | 1 (0%) 91 86 | 72, 115, 156, 202 | 0 |
| 3 | O | 213/233 (91%) | -0.15 | 3 (1%) 75 65 | 81, 126, 165, 227 | 0 |
| 4 | D | 214/470 (45%) | 0.25 | 5 (2%) 60 51 | 82, 148, 198, 280 | 0 |
| 4 | H | 214/470 (45%) | 0.43 | 11 (5%) 28 24 | 81, 146, 196, 265 | 0 |
| 4 | L | 214/470 (45%) | 0.18 | 3 (1%) 75 65 | 74, 135, 181, 258 | 0 |
| 4 | P | 214/470 (45%) | 0.51 | 10 (4%) 31 26 | 79, 159, 203, 291 | 0 |
| All | All | 4704/5920 (79%) | 0.02 | 130 (2%) 53 42 | 58, 145, 234, 343 | 0 |

All (130) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 532 | TYR | 6.3 |
| 1 | E | 501 | LEU | 5.5 |
| 1 | E | 525 | ASP | 5.0 |
| 1 | E | 531 | ALA | 4.9 |
| 1 | E | 535 | VAL | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 519 | LEU | 4.5 |
| 1 | A | 387 | GLY | 4.4 |
| 2 | F | 25 | ALA | 4.3 |
| 1 | A | 501 | LEU | 4.3 |
| 4 | P | 56 | THR | 4.2 |
| 1 | E | 533 | LYS | 4.0 |
| 2 | N | 32 | THR | 4.0 |
| 1 | M | 501 | LEU | 4.0 |
| 1 | E | 520 | GLU | 4.0 |
| 1 | E | 496 | PRO | 4.0 |
| 2 | N | 31 | VAL | 4.0 |
| 1 | A | 499 | ALA | 3.9 |
| 1 | E | 521 | ARG | 3.9 |
| 4 | H | 103 | TRP | 3.9 |
| 2 | N | 25 | ALA | 3.7 |
| 1 | A | 500 | MET | 3.7 |
| 1 | E | 534 | CYS | 3.6 |
| 1 | E | 623 | ASP | 3.6 |
| 1 | I | 496 | PRO | 3.4 |
| 2 | J | 25 | ALA | 3.4 |
| 1 | M | 585 | ASN | 3.3 |
| 1 | E | 591 | ALA | 3.3 |
| 1 | M | 500 | MET | 3.3 |
| 1 | I | 500 | MET | 3.3 |
| 1 | M | 499 | ALA | 3.2 |
| 1 | M | 187 | GLU | 3.2 |
| 4 | H | 104 | PRO | 3.2 |
| 4 | H | 72 | ARG | 3.2 |
| 1 | E | 587 | CYS | 3.1 |
| 1 | E | 502 | ASP | 3.1 |
| 4 | H | 34 | ILE | 3.0 |
| 1 | E | 590 | GLY | 2.9 |
| 1 | I | 525 | ASP | 2.9 |
| 4 | L | 103 | TRP | 2.8 |
| 2 | N | 80 | ALA | 2.8 |
| 1 | I | 585 | ASN | 2.8 |
| 4 | P | 99 | GLY | 2.8 |
| 1 | A | 496 | PRO | 2.8 |
| 1 | E | 589 | GLN | 2.8 |
| 2 | B | 33 | GLN | 2.8 |
| 1 | E | 527 | TRP | 2.8 |
| 3 | O | 2 | ILE | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | B | 25 | ALA | 2.7 |
| 2 | N | 33 | GLN | 2.7 |
| 1 | I | 502 | ASP | 2.6 |
| 4 | L | 104 | PRO | 2.6 |
| 4 | P | 206 | VAL | 2.6 |
| 3 | O | 1 | ASP | 2.6 |
| 1 | I | 501 | LEU | 2.6 |
| 2 | B | 132 | ALA | 2.6 |
| 1 | A | 386 | ALA | 2.6 |
| 1 | E | 593 | ALA | 2.6 |
| 1 | E | 592 | VAL | 2.6 |
| 2 | J | 33 | GLN | 2.5 |
| 1 | E | 644 | LEU | 2.5 |
| 1 | E | 500 | MET | 2.5 |
| 4 | D | 206 | VAL | 2.5 |
| 2 | B | 26 | TYR | 2.5 |
| 1 | E | 560 | VAL | 2.5 |
| 1 | A | 30 | GLU | 2.5 |
| 1 | E | 580 | SER | 2.5 |
| 2 | N | 67 | PRO | 2.5 |
| 4 | D | 56 | THR | 2.5 |
| 4 | D | 78 | THR | 2.4 |
| 4 | H | 55 | GLY | 2.4 |
| 4 | P | 78 | THR | 2.4 |
| 4 | H | 56 | THR | 2.4 |
| 4 | P | 103 | TRP | 2.4 |
| 1 | I | 410 | PHE | 2.4 |
| 2 | B | 66 | SER | 2.4 |
| 1 | A | 585 | ASN | 2.4 |
| 1 | I | 387 | GLY | 2.3 |
| 1 | E | 579 | LEU | 2.3 |
| 1 | E | 588 | SER | 2.3 |
| 4 | D | 214 | LYS | 2.3 |
| 2 | J | 26 | TYR | 2.3 |
| 4 | L | 56 | THR | 2.3 |
| 2 | F | 78 | ARG | 2.3 |
| 1 | I | 563 | SER | 2.3 |
| 1 | E | 563 | SER | 2.3 |
| 1 | E | 585 | ASN | 2.3 |
| 4 | H | 125 | LYS | 2.3 |
| 4 | H | 99 | GLY | 2.3 |
| 2 | B | 67 | PRO | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 530 | PRO | 2.3 |
| 4 | H | 216 | ASP | 2.3 |
| 1 | M | 525 | ASP | 2.3 |
| 3 | K | 2 | ILE | 2.2 |
| 2 | F | 33 | GLN | 2.2 |
| 2 | F | 132 | ALA | 2.2 |
| 4 | P | 104 | PRO | 2.2 |
| 2 | N | 79 | CYS | 2.2 |
| 4 | P | 125 | LYS | 2.2 |
| 1 | M | 591 | ALA | 2.2 |
| 3 | G | 2 | ILE | 2.2 |
| 1 | E | 499 | ALA | 2.2 |
| 4 | H | 74 | ASN | 2.2 |
| 1 | E | 526 | ALA | 2.2 |
| 2 | B | 32 | THR | 2.2 |
| 1 | E | 410 | PHE | 2.2 |
| 1 | E | 360 | LYS | 2.2 |
| 2 | N | 26 | TYR | 2.2 |
| 1 | E | 667 | VAL | 2.2 |
| 1 | M | 496 | PRO | 2.2 |
| 2 | F | 66 | SER | 2.1 |
| 1 | A | 525 | ASP | 2.1 |
| 2 | B | 64 | LEU | 2.1 |
| 4 | D | 50 | MET | 2.1 |
| 2 | N | 132 | ALA | 2.1 |
| 1 | I | 499 | ALA | 2.1 |
| 4 | P | 218 | ARG | 2.1 |
| 1 | M | 410 | PHE | 2.1 |
| 1 | E | 586 | LYS | 2.1 |
| 2 | N | 64 | LEU | 2.1 |
| 4 | H | 207 | ASN | 2.1 |
| 2 | N | 78 | ARG | 2.1 |
| 4 | P | 58 | ASP | 2.1 |
| 1 | I | 519 | LEU | 2.1 |
| 1 | E | 33 | ALA | 2.1 |
| 1 | E | 536 | ASP | 2.1 |
| 3 | O | 120 | PRO | 2.0 |
| 1 | A | 388 | VAL | 2.0 |
| 1 | M | 189 | GLY | 2.0 |
| 4 | P | 210 | PRO | 2.0 |
| 1 | E | 27 | LEU | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.