



Full wwPDB X-ray Structure Validation Report ⓘ

May 31, 2022 – 02:16 PM EDT

PDB ID : 7U8M
Title : Crystal structure of chimeric hemagglutinin cH15/3 in complex with broad protective antibodies 31.a.83 and FluA-20
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2022-03-08
Resolution : 5.39 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:

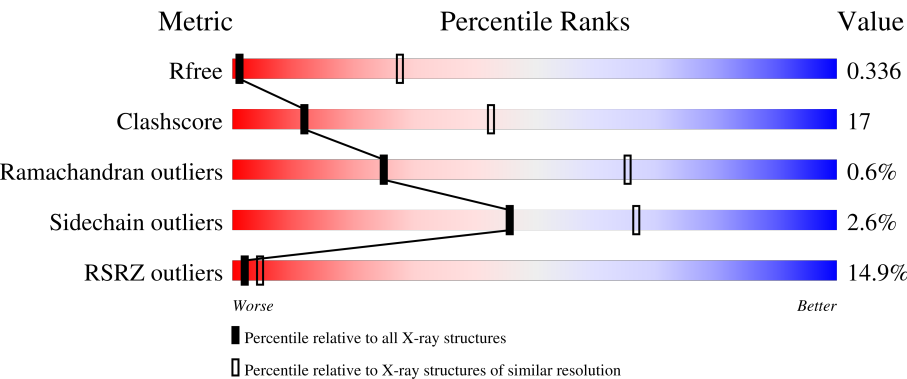
| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.28.1 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.28.1 |

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 5.39 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 | 1207 (7.00-3.80) |
| Clashscore | 141614 | 1016 (6.92-3.86) |
| Ramachandran outliers | 138981 | 1210 (7.00-3.80) |
| Sidechain outliers | 138945 | 1181 (7.00-3.80) |
| RSRZ outliers | 127900 | 1021 (7.04-3.76) |

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 | 333 | <div><div>21%</div><div>57%</div><div>38%</div><div>..</div></div> |
| 1 | C | 333 | <div><div>19%</div><div>57%</div><div>37%</div><div>..</div></div> |
| 1 | G | 333 | <div><div>22%</div><div>55%</div><div>40%</div><div>..</div></div> |
| 2 | B | 176 | <div><div>5%</div><div>86%</div><div>11%</div><div>..</div></div> |
| 2 | D | 176 | <div><div>6%</div><div>91%</div><div>6%</div><div>..</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | I | 176 | |
| 3 | E | 214 | |
| 3 | J | 214 | |
| 3 | L | 214 | |
| 4 | F | 234 | |
| 4 | H | 234 | |
| 4 | K | 234 | |
| 5 | N | 229 | |
| 5 | Q | 229 | |
| 5 | T | 229 | |
| 6 | O | 214 | |
| 6 | R | 214 | |
| 6 | U | 214 | |

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31560 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 hemagglutinin HA1 subunit.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 322 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2482 | 1545 | 444 | 480 | 13 | | | |
| 1 | C | 321 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2474 | 1539 | 443 | 479 | 13 | | | |
| 1 | G | 322 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2482 | 1545 | 444 | 480 | 13 | | | |

- Molecule 2 is a protein called hemagglutinin HA2 subunit.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | B | 173 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1396 | 869 | 247 | 274 | 6 | | | |
| 2 | D | 172 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1390 | 866 | 246 | 272 | 6 | | | |
| 2 | I | 173 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1396 | 869 | 247 | 274 | 6 | | | |

- Molecule 3 is a protein called Antibody 31.a.83 Fab light chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | L | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1643 | 1025 | 281 | 331 | 6 | | | |
| 3 | E | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1643 | 1025 | 281 | 331 | 6 | | | |
| 3 | J | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1643 | 1025 | 281 | 331 | 6 | | | |

- Molecule 4 is a protein called antibody 31.a.83 Fab heavy chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | H | 226 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1699 | 1074 | 280 | 338 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | F | 226 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1699 | 1074 | 280 | 338 | 7 | | | |
| 4 | K | 226 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1699 | 1074 | 280 | 338 | 7 | | | |

- Molecule 5 is a protein called antibody FluA-20 Fab heavy chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | N | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1662 | 1050 | 273 | 332 | 7 | | | |
| 5 | Q | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1658 | 1048 | 272 | 331 | 7 | | | |
| 5 | T | 221 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1656 | 1047 | 272 | 330 | 7 | | | |

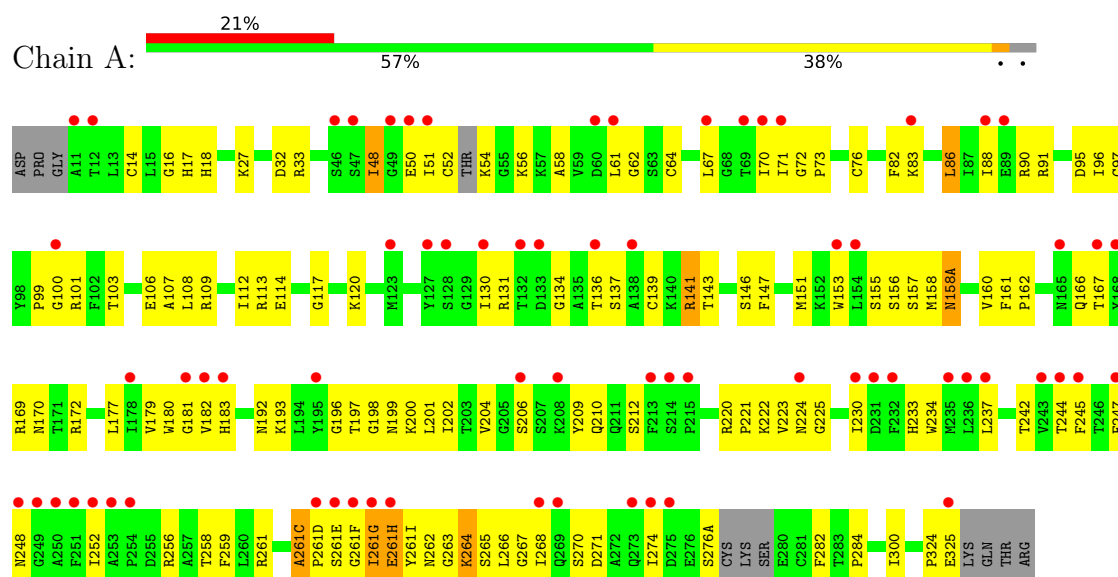
- Molecule 6 is a protein called antibody FluA-20 Fab light chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6 | O | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1646 | 1031 | 281 | 329 | 5 | | | |
| 6 | R | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1646 | 1031 | 281 | 329 | 5 | | | |
| 6 | U | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1646 | 1031 | 281 | 329 | 5 | | | |

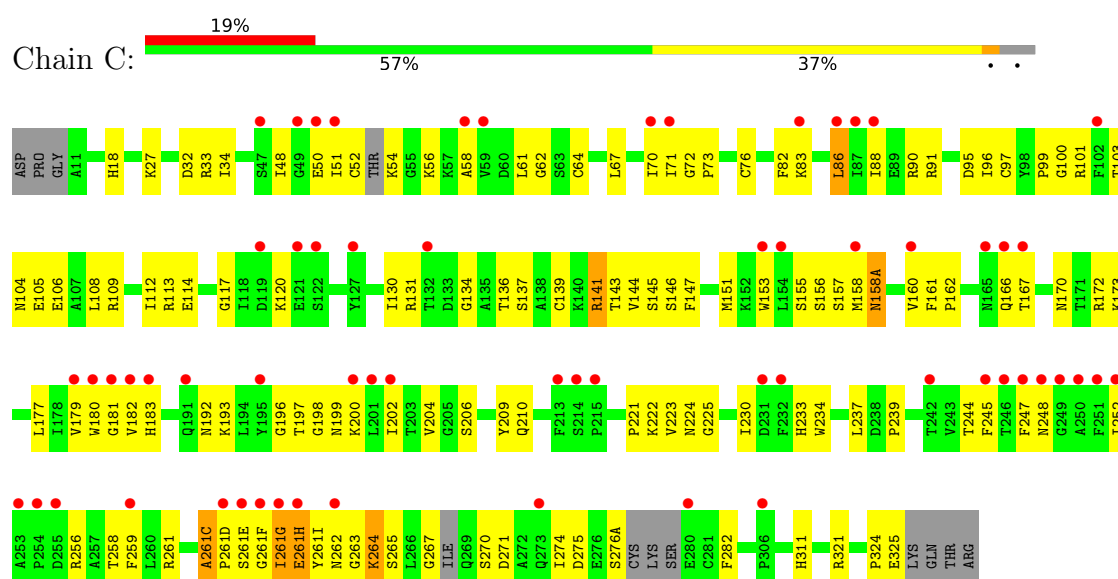
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

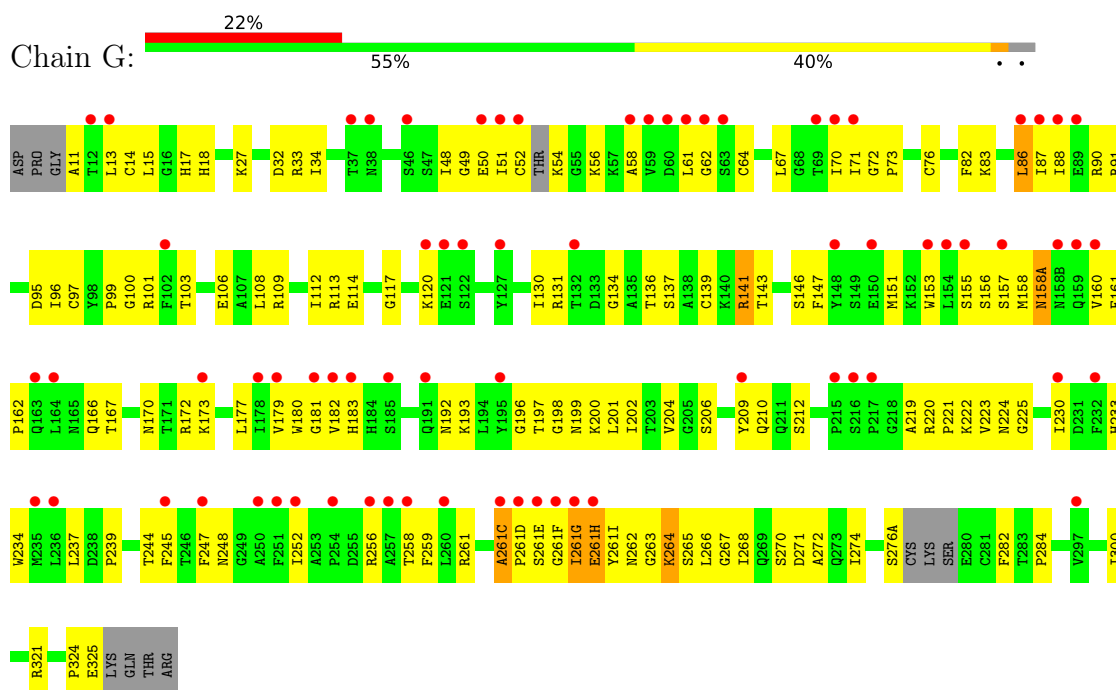
• Molecule 1: hemagglutinin HA1 subunit



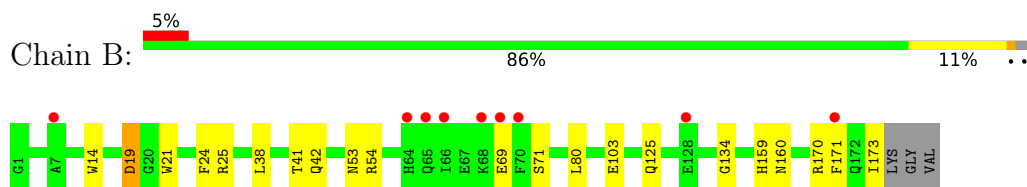
• Molecule 1: hemagglutinin HA1 subunit



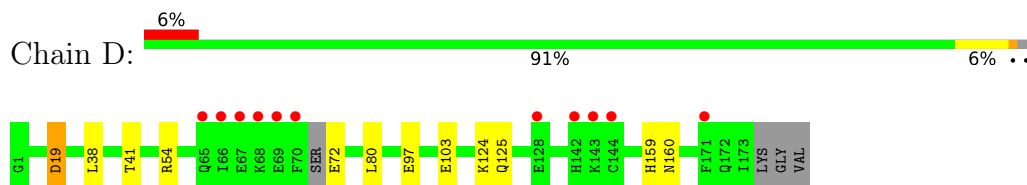
• Molecule 1: hemagglutinin HA1 subunit



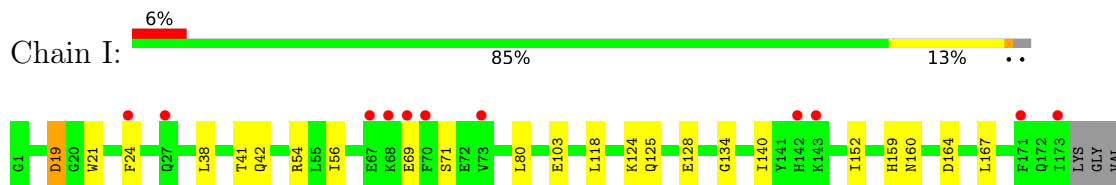
- Molecule 2: hemagglutinin HA2 subunit



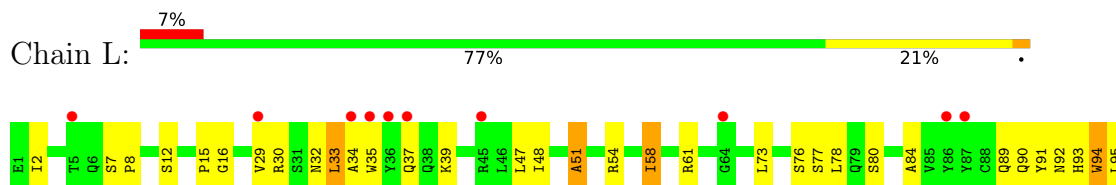
- Molecule 2: hemagglutinin HA2 subunit



- Molecule 2: hemagglutinin HA2 subunit

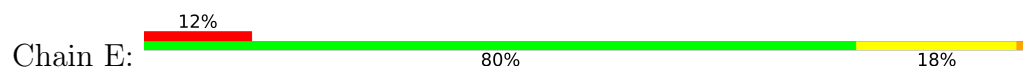


- Molecule 3: Antibody 31.a.83 Fab light chain

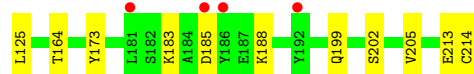
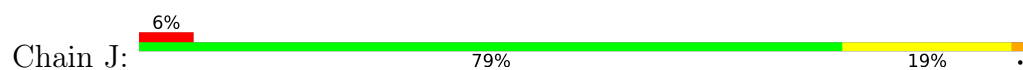




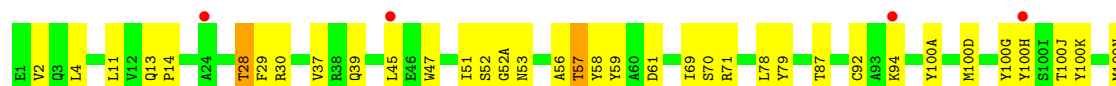
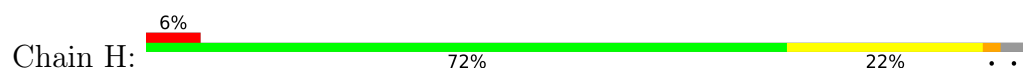
- Molecule 3: Antibody 31.a.83 Fab light chain



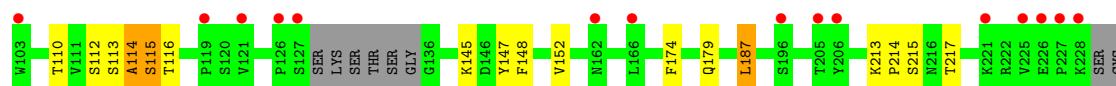
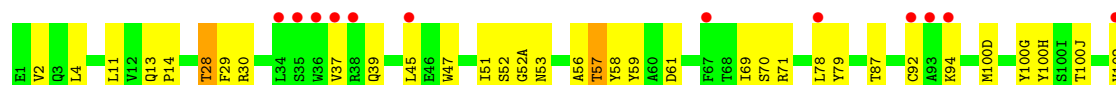
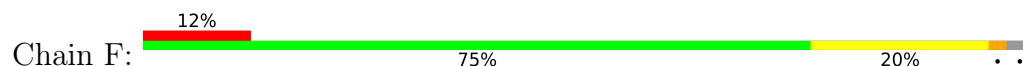
- Molecule 3: Antibody 31.a.83 Fab light chain



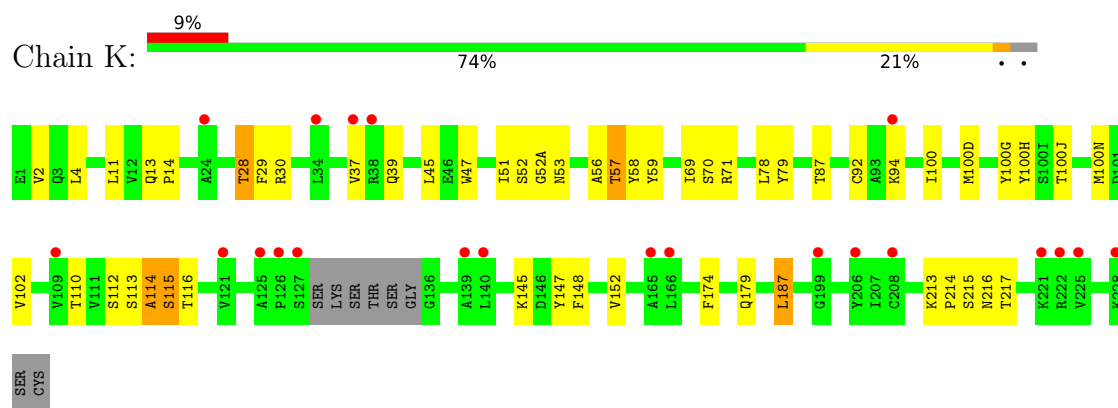
- Molecule 4: antibody 31.a.83 Fab heavy chain



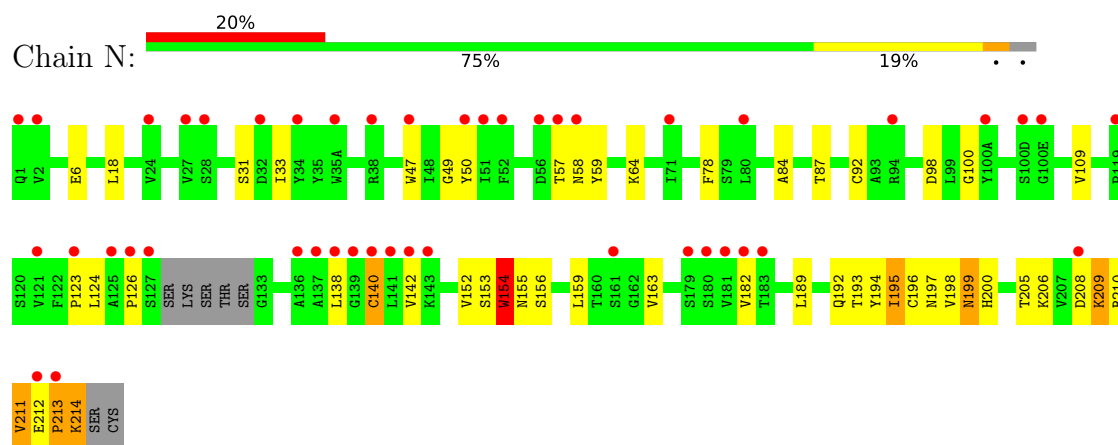
- Molecule 4: antibody 31.a.83 Fab heavy chain



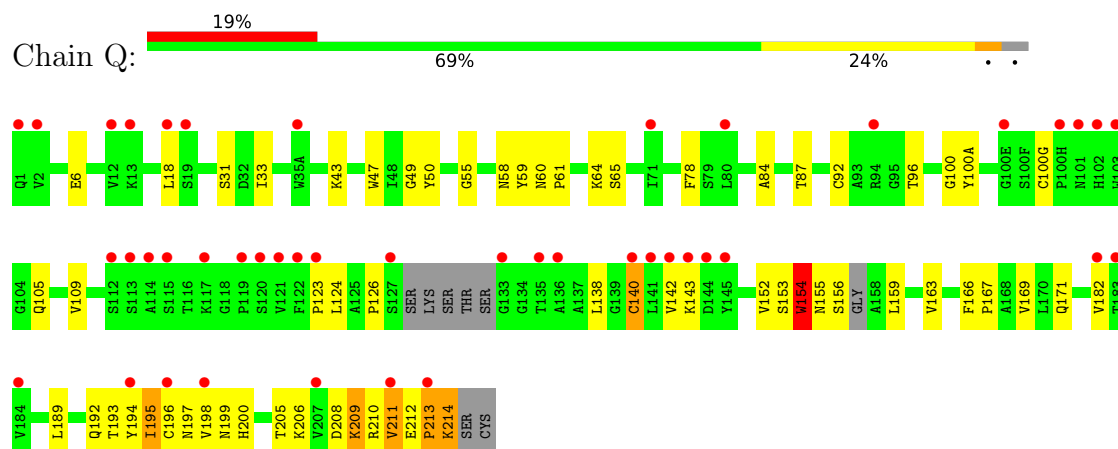
- Molecule 4: antibody 31.a.83 Fab heavy chain



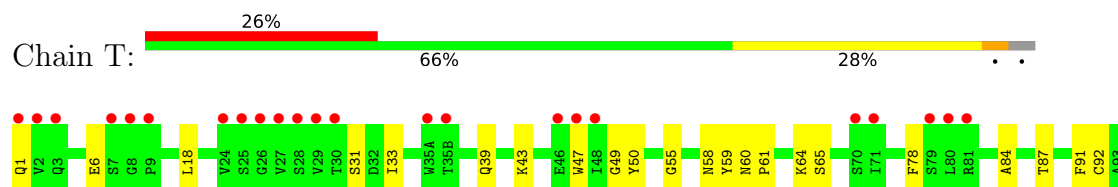
- Molecule 5: antibody FluA-20 Fab heavy chain

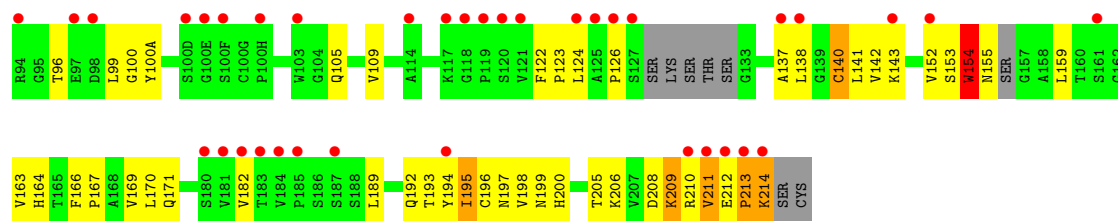


- Molecule 5: antibody FluA-20 Fab heavy chain

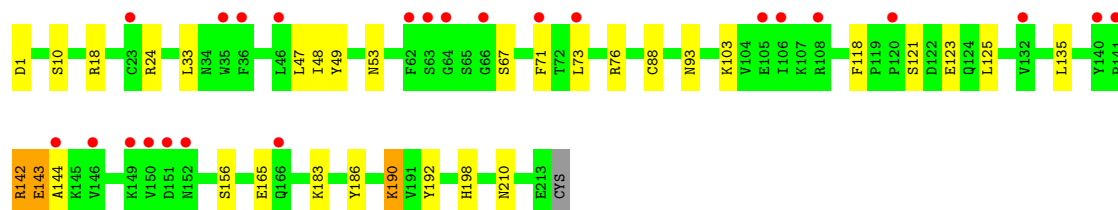
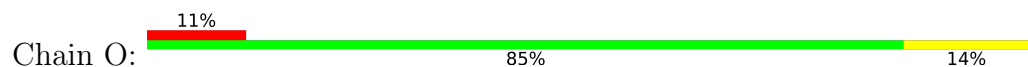


- Molecule 5: antibody FluA-20 Fab heavy chain

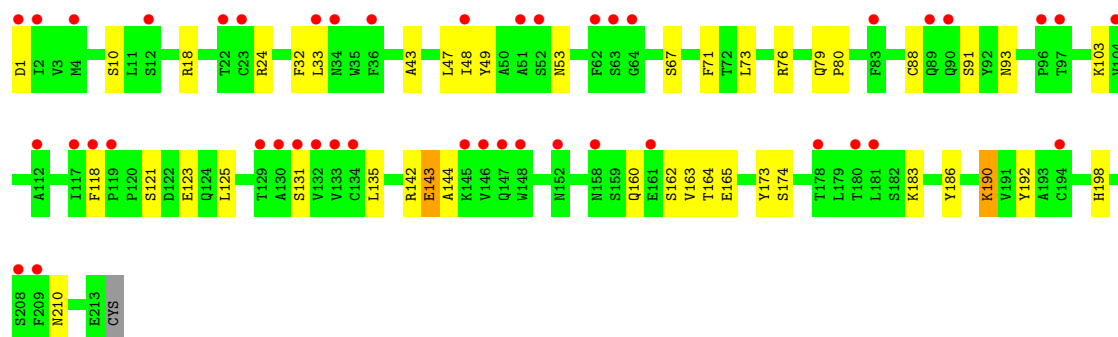
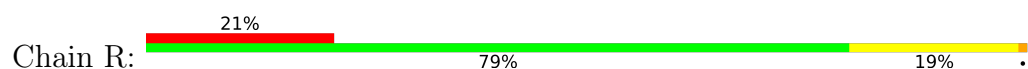




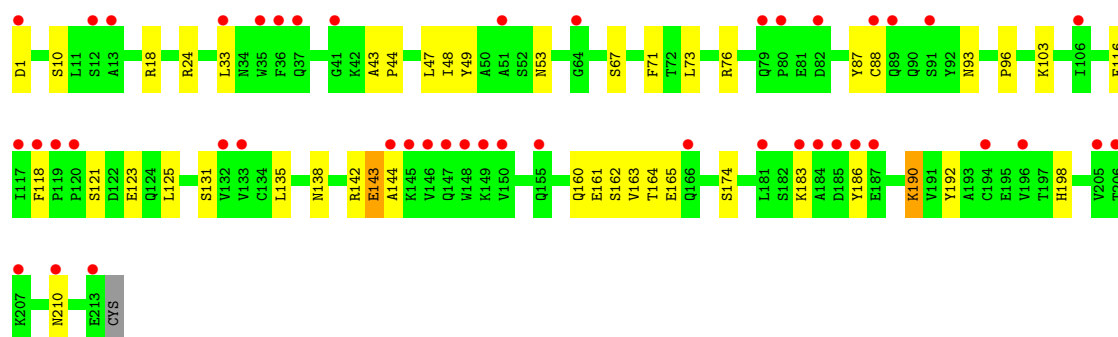
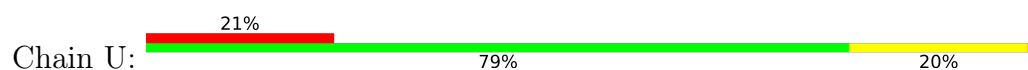
• Molecule 6: antibody FluA-20 Fab light chain



• Molecule 6: antibody FluA-20 Fab light chain



• Molecule 6: antibody FluA-20 Fab light chain



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 1 2 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 272.92Å 155.73Å 156.89Å 90.00° 94.63° 90.00° | Depositor |
| Resolution (Å) | 49.94 – 5.39 49.94 – 5.39 | Depositor EDS |
| % Data completeness (in resolution range) | 95.9 (49.94-5.39) 96.0 (49.94-5.39) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.10 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.46 (at 5.39Å) | Xtriage |
| Refinement program | PHENIX 1.19.2_4158 | Depositor |
| R, R_{free} | 0.304 , 0.342 0.304 , 0.336 | Depositor DCC |
| R_{free} test set | 1073 reflections (4.92%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 248.6 | Xtriage |
| Anisotropy | 0.330 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 294.7 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.81 | EDS |
| Total number of atoms | 31560 | wwPDB-VP |
| Average B, all atoms (Å ²) | 312.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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, 0.333 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 | 0.49 | 0/2531 | 0.75 | 5/3422 (0.1%) |
| 1 | C | 0.49 | 0/2522 | 0.75 | 5/3408 (0.1%) |
| 1 | G | 0.49 | 0/2531 | 0.75 | 5/3422 (0.1%) |
| 2 | B | 0.31 | 0/1420 | 0.46 | 0/1906 |
| 2 | D | 0.31 | 0/1413 | 0.46 | 0/1895 |
| 2 | I | 0.31 | 0/1420 | 0.46 | 0/1906 |
| 3 | E | 0.43 | 0/1677 | 0.55 | 0/2277 |
| 3 | J | 0.42 | 0/1677 | 0.55 | 0/2277 |
| 3 | L | 0.43 | 0/1677 | 0.55 | 0/2277 |
| 4 | F | 0.36 | 0/1741 | 0.56 | 0/2376 |
| 4 | H | 0.36 | 0/1741 | 0.56 | 0/2376 |
| 4 | K | 0.36 | 0/1741 | 0.56 | 0/2376 |
| 5 | N | 0.70 | 1/1704 (0.1%) | 0.91 | 4/2330 (0.2%) |
| 5 | Q | 0.70 | 1/1699 (0.1%) | 0.91 | 3/2322 (0.1%) |
| 5 | T | 0.70 | 1/1697 (0.1%) | 0.91 | 3/2319 (0.1%) |
| 6 | O | 0.66 | 1/1683 (0.1%) | 0.95 | 6/2285 (0.3%) |
| 6 | R | 0.66 | 1/1683 (0.1%) | 0.95 | 6/2285 (0.3%) |
| 6 | U | 0.66 | 1/1683 (0.1%) | 0.94 | 6/2285 (0.3%) |
| All | All | 0.51 | 6/32240 (0.0%) | 0.73 | 43/43744 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 5 | N | 0 | 1 |
| 5 | Q | 0 | 1 |
| 5 | T | 0 | 1 |
| 6 | O | 0 | 1 |
| 6 | R | 0 | 1 |
| 6 | U | 0 | 1 |
| All | All | 0 | 6 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5 | Q | 140 | CYS | CB-SG | -6.67 | 1.71 | 1.82 |
| 5 | T | 140 | CYS | CB-SG | -6.67 | 1.71 | 1.82 |
| 5 | N | 140 | CYS | CB-SG | -6.63 | 1.71 | 1.82 |
| 6 | U | 93 | ASN | C-N | -5.47 | 1.21 | 1.34 |
| 6 | O | 93 | ASN | C-N | -5.47 | 1.21 | 1.34 |
| 6 | R | 93 | ASN | C-N | -5.44 | 1.21 | 1.34 |

All (43) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1 | C | 261(C) | ALA | C-N-CD | -9.17 | 100.43 | 120.60 |
| 1 | G | 261(C) | ALA | C-N-CD | -9.15 | 100.47 | 120.60 |
| 1 | A | 261(C) | ALA | C-N-CD | -9.15 | 100.48 | 120.60 |
| 6 | R | 24 | ARG | NE-CZ-NH1 | 9.14 | 124.87 | 120.30 |
| 6 | O | 24 | ARG | NE-CZ-NH1 | 9.10 | 124.85 | 120.30 |
| 6 | U | 24 | ARG | NE-CZ-NH1 | 9.02 | 124.81 | 120.30 |
| 6 | O | 144 | ALA | N-CA-C | -7.73 | 90.13 | 111.00 |
| 6 | U | 144 | ALA | N-CA-C | -7.73 | 90.14 | 111.00 |
| 6 | R | 144 | ALA | N-CA-C | -7.71 | 90.19 | 111.00 |
| 1 | A | 263 | GLY | N-CA-C | 7.48 | 131.80 | 113.10 |
| 1 | C | 263 | GLY | N-CA-C | 7.46 | 131.74 | 113.10 |
| 1 | G | 263 | GLY | N-CA-C | 7.45 | 131.73 | 113.10 |
| 5 | T | 140 | CYS | CA-CB-SG | 7.02 | 126.63 | 114.00 |
| 5 | Q | 140 | CYS | CA-CB-SG | 7.01 | 126.61 | 114.00 |
| 5 | N | 140 | CYS | CA-CB-SG | 7.00 | 126.61 | 114.00 |
| 1 | G | 72 | GLY | N-CA-C | 6.70 | 129.85 | 113.10 |
| 1 | A | 72 | GLY | N-CA-C | 6.69 | 129.82 | 113.10 |
| 1 | C | 72 | GLY | N-CA-C | 6.68 | 129.81 | 113.10 |
| 1 | G | 264 | LYS | N-CA-C | 6.61 | 128.84 | 111.00 |
| 1 | C | 264 | LYS | N-CA-C | 6.61 | 128.84 | 111.00 |
| 1 | A | 264 | LYS | N-CA-C | 6.59 | 128.80 | 111.00 |
| 6 | U | 142 | ARG | CG-CD-NE | 6.06 | 124.53 | 111.80 |
| 6 | O | 24 | ARG | NE-CZ-NH2 | -6.04 | 117.28 | 120.30 |
| 6 | U | 24 | ARG | NE-CZ-NH2 | -6.04 | 117.28 | 120.30 |
| 6 | O | 142 | ARG | CG-CD-NE | 6.03 | 124.46 | 111.80 |
| 6 | R | 24 | ARG | NE-CZ-NH2 | -6.01 | 117.29 | 120.30 |
| 6 | R | 142 | ARG | CG-CD-NE | 5.99 | 124.38 | 111.80 |
| 6 | R | 47 | LEU | CA-CB-CG | 5.81 | 128.67 | 115.30 |
| 6 | U | 47 | LEU | CA-CB-CG | 5.77 | 128.58 | 115.30 |
| 6 | O | 47 | LEU | CA-CB-CG | 5.77 | 128.57 | 115.30 |
| 5 | N | 138 | LEU | CB-CG-CD2 | 5.73 | 120.74 | 111.00 |
| 5 | T | 138 | LEU | CB-CG-CD2 | 5.71 | 120.71 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 5 | Q | 138 | LEU | CB-CG-CD2 | 5.70 | 120.69 | 111.00 |
| 1 | A | 261(H) | GLU | N-CA-C | -5.65 | 95.74 | 111.00 |
| 1 | C | 261(H) | GLU | N-CA-C | -5.64 | 95.78 | 111.00 |
| 1 | G | 261(H) | GLU | N-CA-C | -5.64 | 95.78 | 111.00 |
| 5 | T | 154 | TRP | O-C-N | -5.63 | 113.69 | 122.70 |
| 5 | N | 154 | TRP | O-C-N | -5.63 | 113.70 | 122.70 |
| 5 | Q | 154 | TRP | O-C-N | -5.59 | 113.76 | 122.70 |
| 6 | U | 190 | LYS | CG-CD-CE | -5.33 | 95.90 | 111.90 |
| 6 | O | 190 | LYS | CG-CD-CE | -5.31 | 95.96 | 111.90 |
| 6 | R | 190 | LYS | CG-CD-CE | -5.31 | 95.97 | 111.90 |
| 5 | N | 199 | ASN | CB-CA-C | 5.02 | 120.44 | 110.40 |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 5 | N | 154 | TRP | Mainchain |
| 6 | O | 143 | GLU | Mainchain |
| 5 | Q | 154 | TRP | Mainchain |
| 6 | R | 143 | GLU | Mainchain |
| 5 | T | 154 | TRP | Mainchain |
| 6 | U | 143 | GLU | Mainchain |

5.2 Too-close contacts [i](#)

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 | 2482 | 0 | 2431 | 162 | 0 |
| 1 | C | 2474 | 0 | 2418 | 148 | 0 |
| 1 | G | 2482 | 0 | 2430 | 183 | 0 |
| 2 | B | 1396 | 0 | 1331 | 49 | 0 |
| 2 | D | 1390 | 0 | 1324 | 26 | 0 |
| 2 | I | 1396 | 0 | 1330 | 40 | 0 |
| 3 | E | 1643 | 0 | 1592 | 41 | 0 |
| 3 | J | 1643 | 0 | 1592 | 45 | 0 |
| 3 | L | 1643 | 0 | 1592 | 46 | 0 |
| 4 | F | 1699 | 0 | 1650 | 67 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | H | 1699 | 0 | 1650 | 85 | 0 |
| 4 | K | 1699 | 0 | 1650 | 56 | 0 |
| 5 | N | 1662 | 0 | 1618 | 59 | 0 |
| 5 | Q | 1658 | 0 | 1614 | 90 | 0 |
| 5 | T | 1656 | 0 | 1612 | 121 | 0 |
| 6 | O | 1646 | 0 | 1608 | 38 | 0 |
| 6 | R | 1646 | 0 | 1608 | 64 | 0 |
| 6 | U | 1646 | 0 | 1608 | 74 | 0 |
| All | All | 31560 | 0 | 30658 | 1078 | 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 17.

All (1078) 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:G:51:ILE:HD11 | 1:G:268:ILE:CG2 | 1.37 | 1.51 |
| 1:A:106:GLU:CB | 2:B:71:SER:HB2 | 1.47 | 1.43 |
| 1:C:101:ARG:NE | 5:N:100:GLY:HA2 | 1.40 | 1.32 |
| 1:G:106:GLU:CB | 2:I:71:SER:HB2 | 1.60 | 1.31 |
| 1:G:106:GLU:HB3 | 2:I:71:SER:CB | 1.60 | 1.31 |
| 5:T:169:VAL:CG1 | 6:U:162:SER:HB3 | 1.61 | 1.30 |
| 1:A:106:GLU:HB3 | 2:B:71:SER:CB | 1.62 | 1.27 |
| 1:C:101:ARG:HE | 5:N:100:GLY:CA | 1.50 | 1.23 |
| 1:G:106:GLU:CG | 2:I:71:SER:HB3 | 1.67 | 1.23 |
| 5:T:166:PHE:CD1 | 6:U:164:THR:HG23 | 1.74 | 1.21 |
| 1:A:33:ARG:HH22 | 3:J:2:ILE:CD1 | 1.56 | 1.17 |
| 2:I:42:GLN:OE1 | 4:K:100(G):TYR:HB3 | 1.43 | 1.16 |
| 1:C:51:ILE:HB | 1:C:86:LEU:CD2 | 1.76 | 1.16 |
| 1:G:220:ARG:HG2 | 5:T:96:THR:HG21 | 1.17 | 1.15 |
| 5:Q:212:GLU:HG3 | 5:Q:213:PRO:HD2 | 1.29 | 1.14 |
| 1:G:51:ILE:HD11 | 1:G:268:ILE:HG23 | 1.17 | 1.14 |
| 5:T:169:VAL:HG13 | 6:U:162:SER:HB3 | 1.17 | 1.14 |
| 1:A:221:PRO:HB2 | 6:R:49:TYR:CE2 | 1.80 | 1.14 |
| 1:A:268:ILE:HB | 1:A:284:PRO:O | 1.46 | 1.13 |
| 1:G:51:ILE:HB | 1:G:86:LEU:HG | 1.31 | 1.13 |
| 5:N:212:GLU:HG3 | 5:N:213:PRO:HD2 | 1.29 | 1.13 |
| 1:C:51:ILE:HD12 | 1:C:86:LEU:HD13 | 1.27 | 1.12 |
| 1:C:51:ILE:CB | 1:C:86:LEU:HD22 | 1.78 | 1.12 |
| 5:T:212:GLU:HG3 | 5:T:213:PRO:HD2 | 1.29 | 1.12 |
| 1:G:86:LEU:HD22 | 1:G:86:LEU:C | 1.70 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:G:51:ILE:HG13 | 1:G:268:ILE:HD13 | 1.29 | 1.12 |
| 1:G:52:CYS:O | 1:G:56:LYS:HG3 | 1.48 | 1.11 |
| 1:A:106:GLU:HG3 | 2:B:71:SER:HB3 | 1.28 | 1.10 |
| 1:G:106:GLU:CG | 2:I:71:SER:CB | 2.30 | 1.10 |
| 1:G:51:ILE:HD11 | 1:G:268:ILE:HG21 | 1.14 | 1.09 |
| 1:A:33:ARG:HH22 | 3:J:2:ILE:HD12 | 1.17 | 1.09 |
| 1:C:101:ARG:CZ | 5:N:100:GLY:HA2 | 1.82 | 1.09 |
| 2:B:41:THR:HG21 | 4:H:100(G):TYR:CE1 | 1.88 | 1.09 |
| 5:T:124:LEU:HB3 | 6:U:118:PHE:CE1 | 1.87 | 1.09 |
| 1:A:33:ARG:NH2 | 3:J:2:ILE:HD12 | 1.67 | 1.08 |
| 1:G:268:ILE:HB | 1:G:284:PRO:O | 1.54 | 1.08 |
| 1:G:86:LEU:C | 1:G:86:LEU:CD2 | 2.20 | 1.08 |
| 1:G:51:ILE:CD1 | 1:G:268:ILE:CG2 | 2.33 | 1.06 |
| 1:C:221:PRO:HB2 | 6:O:49:TYR:CE2 | 1.89 | 1.06 |
| 2:D:38:LEU:CD2 | 4:F:53:ASN:HB3 | 1.86 | 1.05 |
| 3:L:2:ILE:CD1 | 1:C:33:ARG:HH22 | 1.67 | 1.05 |
| 5:Q:169:VAL:CG1 | 6:R:162:SER:HB2 | 1.86 | 1.05 |
| 2:D:41:THR:HG21 | 4:F:100(G):TYR:CE1 | 1.90 | 1.05 |
| 4:F:114:ALA:HB3 | 4:F:148:PHE:CE2 | 1.94 | 1.03 |
| 1:G:106:GLU:HG3 | 2:I:71:SER:HB3 | 1.38 | 1.02 |
| 4:H:114:ALA:HB3 | 4:H:148:PHE:CE2 | 1.94 | 1.02 |
| 1:G:106:GLU:CB | 2:I:71:SER:CB | 2.25 | 1.02 |
| 4:K:114:ALA:HB3 | 4:K:148:PHE:CE2 | 1.94 | 1.02 |
| 3:L:2:ILE:HD12 | 1:C:33:ARG:HH22 | 1.21 | 1.02 |
| 1:C:173:LYS:HE2 | 5:T:55:GLY:HA3 | 1.42 | 1.01 |
| 5:Q:166:PHE:CD1 | 6:R:164:THR:HG23 | 1.94 | 1.01 |
| 1:G:52:CYS:C | 1:G:56:LYS:HG3 | 1.80 | 1.01 |
| 1:G:220:ARG:HG2 | 5:T:96:THR:CG2 | 1.90 | 1.00 |
| 1:A:268:ILE:HG22 | 1:A:284:PRO:HA | 1.43 | 1.00 |
| 4:H:114:ALA:CB | 4:H:148:PHE:CE2 | 2.45 | 1.00 |
| 4:F:114:ALA:CB | 4:F:148:PHE:CE2 | 2.45 | 1.00 |
| 4:K:114:ALA:CB | 4:K:148:PHE:CE2 | 2.45 | 1.00 |
| 3:L:93:HIS:HB2 | 1:C:33:ARG:HH11 | 1.25 | 0.99 |
| 1:G:51:ILE:CD1 | 1:G:268:ILE:HG23 | 1.91 | 0.99 |
| 1:A:51:ILE:HD11 | 1:A:268:ILE:CG2 | 1.92 | 0.99 |
| 1:A:106:GLU:CG | 2:B:71:SER:CB | 2.40 | 0.99 |
| 2:B:38:LEU:HA | 4:H:100(G):TYR:OH | 1.62 | 0.99 |
| 3:E:2:ILE:HD12 | 1:G:33:ARG:HH22 | 1.28 | 0.98 |
| 1:G:49:GLY:HA3 | 1:G:272:ALA:HB3 | 1.43 | 0.98 |
| 5:N:214:LYS:HD3 | 5:N:214:LYS:H | 1.28 | 0.98 |
| 2:B:38:LEU:O | 4:H:100(G):TYR:HE2 | 1.46 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:L:2:ILE:HD12 | 1:C:33:ARG:NH2 | 1.78 | 0.98 |
| 5:Q:212:GLU:CG | 5:Q:213:PRO:HD2 | 1.93 | 0.98 |
| 5:N:212:GLU:CG | 5:N:213:PRO:HD2 | 1.93 | 0.97 |
| 5:T:61:PRO:HA | 5:T:64:LYS:HE2 | 1.41 | 0.97 |
| 1:A:51:ILE:HB | 1:A:86:LEU:HD22 | 1.45 | 0.97 |
| 1:C:101:ARG:HE | 5:N:100:GLY:HA2 | 0.91 | 0.97 |
| 5:Q:214:LYS:H | 5:Q:214:LYS:HD3 | 1.28 | 0.97 |
| 1:A:106:GLU:CB | 2:B:71:SER:CB | 2.29 | 0.97 |
| 5:T:212:GLU:CG | 5:T:213:PRO:HD2 | 1.93 | 0.97 |
| 5:T:214:LYS:H | 5:T:214:LYS:HD3 | 1.28 | 0.96 |
| 1:G:86:LEU:HD22 | 1:G:86:LEU:O | 1.64 | 0.96 |
| 1:G:106:GLU:HB3 | 2:I:71:SER:HB2 | 0.96 | 0.95 |
| 1:G:261(E):SER:OG | 5:Q:64:LYS:HE2 | 1.67 | 0.95 |
| 1:A:106:GLU:CG | 2:B:71:SER:HB3 | 1.94 | 0.94 |
| 1:G:49:GLY:HA3 | 1:G:272:ALA:CB | 1.97 | 0.94 |
| 1:A:101:ARG:HG3 | 5:Q:100:GLY:HA2 | 1.49 | 0.93 |
| 5:T:124:LEU:HD12 | 6:U:118:PHE:CG | 2.03 | 0.93 |
| 2:B:38:LEU:CD2 | 4:H:53:ASN:HB3 | 1.98 | 0.93 |
| 1:A:101:ARG:HG3 | 5:Q:100:GLY:CA | 1.99 | 0.93 |
| 3:E:2:ILE:CD1 | 1:G:33:ARG:HH22 | 1.82 | 0.93 |
| 1:G:51:ILE:CG1 | 1:G:268:ILE:HD13 | 1.99 | 0.92 |
| 5:T:166:PHE:CD1 | 6:U:164:THR:CG2 | 2.52 | 0.92 |
| 1:G:51:ILE:CD1 | 1:G:268:ILE:HG21 | 1.97 | 0.91 |
| 5:T:169:VAL:HG13 | 6:U:162:SER:CB | 2.01 | 0.91 |
| 5:T:124:LEU:HB3 | 6:U:118:PHE:CZ | 2.04 | 0.91 |
| 5:T:154:TRP:O | 5:T:155:ASN:HB2 | 1.70 | 0.90 |
| 5:Q:124:LEU:HB3 | 6:R:118:PHE:CE1 | 2.07 | 0.90 |
| 1:G:51:ILE:HB | 1:G:86:LEU:CG | 2.02 | 0.90 |
| 1:C:221:PRO:HB2 | 6:O:49:TYR:CD2 | 2.07 | 0.89 |
| 1:C:51:ILE:CD1 | 1:C:86:LEU:HD13 | 2.01 | 0.89 |
| 5:Q:169:VAL:HG13 | 6:R:162:SER:HB2 | 1.51 | 0.89 |
| 1:G:86:LEU:HD23 | 1:G:87:ILE:N | 1.88 | 0.88 |
| 5:Q:154:TRP:O | 5:Q:155:ASN:HB2 | 1.69 | 0.88 |
| 1:G:221:PRO:HB2 | 6:U:49:TYR:CE2 | 2.08 | 0.88 |
| 5:N:154:TRP:O | 5:N:155:ASN:HB2 | 1.70 | 0.88 |
| 1:A:51:ILE:HD11 | 1:A:268:ILE:HG21 | 1.53 | 0.88 |
| 2:B:38:LEU:O | 4:H:100(G):TYR:CE2 | 2.27 | 0.88 |
| 1:C:51:ILE:HD12 | 1:C:86:LEU:CD1 | 2.03 | 0.88 |
| 5:T:61:PRO:CA | 5:T:64:LYS:HE2 | 2.04 | 0.88 |
| 5:T:159:LEU:HD22 | 5:T:194:TYR:CE1 | 2.09 | 0.88 |
| 5:T:166:PHE:HE1 | 6:U:174:SER:C | 1.76 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 5:Q:166:PHE:CE1 | 6:R:164:THR:HG23 | 2.09 | 0.87 |
| 2:B:41:THR:HB | 4:H:100(G):TYR:CZ | 2.09 | 0.87 |
| 5:N:159:LEU:HD22 | 5:N:194:TYR:CE1 | 2.09 | 0.87 |
| 5:Q:159:LEU:HD22 | 5:Q:194:TYR:CE1 | 2.09 | 0.87 |
| 1:C:222:LYS:O | 6:O:53:ASN:HB3 | 1.75 | 0.86 |
| 6:R:190:LYS:HZ1 | 6:R:210:ASN:HA | 1.40 | 0.86 |
| 1:G:106:GLU:HG2 | 2:I:71:SER:HB3 | 1.57 | 0.86 |
| 5:T:166:PHE:CE1 | 6:U:164:THR:HG23 | 2.10 | 0.86 |
| 1:C:101:ARG:NH2 | 5:N:100:GLY:HA2 | 1.91 | 0.86 |
| 1:C:261:ARG:NH1 | 1:C:261(H):GLU:HG3 | 1.91 | 0.85 |
| 3:E:2:ILE:HD12 | 1:G:33:ARG:NH2 | 1.89 | 0.85 |
| 1:G:51:ILE:CB | 1:G:86:LEU:HG | 2.07 | 0.85 |
| 5:Q:59:TYR:HB2 | 5:Q:64:LYS:HG2 | 1.57 | 0.85 |
| 1:G:261:ARG:NH1 | 1:G:261(H):GLU:HG3 | 1.91 | 0.84 |
| 1:G:220:ARG:CG | 5:T:96:THR:HG21 | 2.03 | 0.84 |
| 4:H:100(J):THR:HG23 | 4:H:100(K):TYR:CE1 | 2.12 | 0.84 |
| 1:G:58:ALA:CB | 1:G:86:LEU:HD13 | 2.08 | 0.84 |
| 2:B:41:THR:CG2 | 4:H:100(G):TYR:CE1 | 2.61 | 0.83 |
| 1:A:261:ARG:NH1 | 1:A:261(H):GLU:HG3 | 1.91 | 0.83 |
| 5:N:212:GLU:OE2 | 5:N:213:PRO:HD3 | 1.78 | 0.83 |
| 6:O:190:LYS:HZ1 | 6:O:210:ASN:HA | 1.43 | 0.83 |
| 5:T:212:GLU:OE2 | 5:T:213:PRO:HD3 | 1.78 | 0.83 |
| 2:D:41:THR:HG21 | 4:F:100(G):TYR:CZ | 2.14 | 0.83 |
| 1:G:52:CYS:C | 1:G:56:LYS:CG | 2.47 | 0.83 |
| 5:Q:212:GLU:OE2 | 5:Q:213:PRO:HD3 | 1.78 | 0.83 |
| 5:T:166:PHE:HZ | 6:U:174:SER:HB3 | 1.42 | 0.83 |
| 6:U:190:LYS:HZ1 | 6:U:210:ASN:HA | 1.43 | 0.83 |
| 5:T:59:TYR:HB2 | 5:T:64:LYS:HG2 | 1.58 | 0.82 |
| 1:G:268:ILE:HG22 | 1:G:284:PRO:HA | 1.61 | 0.82 |
| 2:D:38:LEU:HD21 | 4:F:53:ASN:HB3 | 1.60 | 0.81 |
| 5:T:166:PHE:HA | 6:U:164:THR:HG22 | 1.62 | 0.81 |
| 1:A:221:PRO:CB | 6:R:49:TYR:CE2 | 2.63 | 0.81 |
| 1:A:33:ARG:CZ | 3:J:2:ILE:HD12 | 2.11 | 0.81 |
| 1:C:221:PRO:HG2 | 6:O:49:TYR:CZ | 2.16 | 0.81 |
| 5:T:169:VAL:CG1 | 6:U:162:SER:CB | 2.53 | 0.81 |
| 1:A:131:ARG:HG3 | 1:A:157:SER:HA | 1.63 | 0.81 |
| 1:A:48:ILE:HD13 | 1:A:50:GLU:OE1 | 1.81 | 0.80 |
| 1:C:101:ARG:NE | 5:N:100:GLY:CA | 2.22 | 0.80 |
| 1:C:131:ARG:HG3 | 1:C:157:SER:HA | 1.63 | 0.80 |
| 1:A:51:ILE:HD11 | 1:A:268:ILE:HG23 | 1.63 | 0.80 |
| 3:L:93:HIS:HB2 | 1:C:33:ARG:NH1 | 1.96 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:A:261(F):GLY:O | 1:A:261(G):ILE:HG13 | 1.82 | 0.79 |
| 2:B:42:GLN:HB2 | 4:H:100(G):TYR:HD2 | 1.47 | 0.79 |
| 1:G:86:LEU:CD2 | 1:G:87:ILE:N | 2.45 | 0.79 |
| 1:C:51:ILE:HB | 1:C:86:LEU:HD22 | 0.86 | 0.79 |
| 1:G:131:ARG:HG3 | 1:G:157:SER:HA | 1.63 | 0.79 |
| 1:G:261(F):GLY:O | 1:G:261(G):ILE:HG13 | 1.82 | 0.79 |
| 1:A:48:ILE:CD1 | 1:A:50:GLU:OE1 | 2.31 | 0.79 |
| 5:T:169:VAL:HG11 | 6:U:162:SER:HB3 | 1.60 | 0.78 |
| 5:Q:166:PHE:CD1 | 6:R:164:THR:CG2 | 2.65 | 0.78 |
| 5:T:166:PHE:CZ | 6:U:174:SER:HB3 | 2.19 | 0.78 |
| 2:I:42:GLN:OE1 | 4:K:100(G):TYR:CB | 2.30 | 0.78 |
| 6:R:190:LYS:NZ | 6:R:190:LYS:O | 2.17 | 0.78 |
| 1:C:261(F):GLY:O | 1:C:261(G):ILE:HG13 | 1.82 | 0.77 |
| 1:C:311:HIS:CE1 | 2:D:97:GLU:OE1 | 2.37 | 0.77 |
| 6:O:190:LYS:O | 6:O:190:LYS:NZ | 2.17 | 0.77 |
| 6:U:190:LYS:NZ | 6:U:190:LYS:O | 2.17 | 0.77 |
| 1:G:58:ALA:HB2 | 1:G:86:LEU:HD13 | 1.67 | 0.77 |
| 1:G:106:GLU:HG2 | 2:I:71:SER:CB | 2.09 | 0.77 |
| 1:A:33:ARG:NH2 | 3:J:2:ILE:CD1 | 2.33 | 0.77 |
| 5:T:159:LEU:HD22 | 5:T:194:TYR:HE1 | 1.50 | 0.76 |
| 5:T:124:LEU:HD12 | 6:U:118:PHE:CD2 | 2.20 | 0.76 |
| 1:A:261(E):SER:O | 5:N:59:TYR:CD2 | 2.37 | 0.76 |
| 5:T:166:PHE:CZ | 6:U:174:SER:CB | 2.69 | 0.76 |
| 4:K:14:PRO:HD3 | 4:K:112:SER:O | 1.86 | 0.76 |
| 5:N:153:SER:HB2 | 5:N:197:ASN:ND2 | 2.01 | 0.75 |
| 1:G:261(E):SER:OG | 5:Q:64:LYS:CE | 2.35 | 0.75 |
| 1:C:170:ASN:HB2 | 1:C:237:LEU:HD23 | 1.68 | 0.75 |
| 1:G:51:ILE:HB | 1:G:86:LEU:CD1 | 2.16 | 0.75 |
| 5:T:153:SER:HB2 | 5:T:197:ASN:ND2 | 2.01 | 0.75 |
| 1:G:170:ASN:HB2 | 1:G:237:LEU:HD23 | 1.68 | 0.75 |
| 4:H:52:SER:HB3 | 4:H:100(H):TYR:HD1 | 1.52 | 0.75 |
| 1:G:51:ILE:HG13 | 1:G:268:ILE:CD1 | 2.15 | 0.75 |
| 2:B:38:LEU:HD23 | 4:H:53:ASN:HB3 | 1.68 | 0.75 |
| 3:E:32:ASN:HB3 | 3:E:91:TYR:HB3 | 1.69 | 0.75 |
| 5:T:167:PRO:HD3 | 6:U:164:THR:HA | 1.67 | 0.75 |
| 4:F:52:SER:HB3 | 4:F:100(H):TYR:HD1 | 1.52 | 0.74 |
| 5:Q:153:SER:HB2 | 5:Q:197:ASN:ND2 | 2.01 | 0.74 |
| 1:A:222:LYS:HE2 | 1:A:225:GLY:HA2 | 1.69 | 0.74 |
| 3:L:32:ASN:HB3 | 3:L:91:TYR:HB3 | 1.69 | 0.74 |
| 4:H:14:PRO:HD3 | 4:H:112:SER:O | 1.86 | 0.74 |
| 1:G:51:ILE:O | 1:G:86:LEU:HD12 | 1.87 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 5:T:167:PRO:CD | 6:U:164:THR:HA | 2.17 | 0.74 |
| 4:F:14:PRO:HD3 | 4:F:112:SER:O | 1.86 | 0.74 |
| 5:T:143:LYS:HE3 | 6:U:131:SER:OG | 1.87 | 0.74 |
| 1:C:221:PRO:CB | 6:O:49:TYR:CE2 | 2.69 | 0.74 |
| 4:K:52:SER:HB3 | 4:K:100(H):TYR:HD1 | 1.52 | 0.74 |
| 3:J:32:ASN:HB3 | 3:J:91:TYR:HB3 | 1.69 | 0.74 |
| 5:N:214:LYS:H | 5:N:214:LYS:CD | 2.00 | 0.74 |
| 1:A:170:ASN:HB2 | 1:A:237:LEU:HD23 | 1.68 | 0.73 |
| 1:G:222:LYS:HE2 | 1:G:225:GLY:HA2 | 1.70 | 0.73 |
| 1:C:222:LYS:HE2 | 1:C:225:GLY:HA2 | 1.69 | 0.73 |
| 5:T:171:GLN:HA | 6:U:160:GLN:OE1 | 1.89 | 0.73 |
| 1:A:51:ILE:HD13 | 1:A:266:LEU:HD23 | 1.70 | 0.73 |
| 5:Q:124:LEU:HD12 | 6:R:118:PHE:CG | 2.24 | 0.73 |
| 5:Q:159:LEU:HD22 | 5:Q:194:TYR:HE1 | 1.50 | 0.72 |
| 1:G:86:LEU:C | 1:G:86:LEU:HD23 | 2.09 | 0.72 |
| 5:T:214:LYS:H | 5:T:214:LYS:CD | 2.00 | 0.72 |
| 1:G:27:LYS:NZ | 1:G:32:ASP:OD1 | 2.23 | 0.72 |
| 1:C:221:PRO:CB | 6:O:49:TYR:CD2 | 2.73 | 0.72 |
| 1:C:27:LYS:NZ | 1:C:32:ASP:OD1 | 2.23 | 0.72 |
| 2:B:42:GLN:HB2 | 4:H:100(G):TYR:CD2 | 2.24 | 0.71 |
| 1:A:131:ARG:HB2 | 1:A:155:SER:HB2 | 1.71 | 0.71 |
| 1:A:220:ARG:HG2 | 5:Q:96:THR:HG21 | 1.71 | 0.71 |
| 4:H:28:THR:HG21 | 4:H:94:LYS:HZ1 | 1.55 | 0.71 |
| 5:N:159:LEU:HD22 | 5:N:194:TYR:HE1 | 1.50 | 0.71 |
| 5:N:208:ASP:O | 5:N:209:LYS:HD2 | 1.91 | 0.71 |
| 4:K:11:LEU:HD11 | 4:K:148:PHE:HE2 | 1.54 | 0.71 |
| 1:C:90:ARG:NH1 | 1:C:270:SER:O | 2.24 | 0.71 |
| 1:C:131:ARG:HB2 | 1:C:155:SER:HB2 | 1.71 | 0.71 |
| 2:D:41:THR:CG2 | 4:F:100(G):TYR:CZ | 2.74 | 0.71 |
| 5:T:208:ASP:O | 5:T:209:LYS:HD2 | 1.91 | 0.71 |
| 1:C:104:ASN:OD1 | 2:D:72:GLU:HG3 | 1.90 | 0.71 |
| 5:Q:208:ASP:O | 5:Q:209:LYS:HD2 | 1.91 | 0.71 |
| 1:A:27:LYS:NZ | 1:A:32:ASP:OD1 | 2.23 | 0.71 |
| 1:A:90:ARG:NH1 | 1:A:270:SER:O | 2.24 | 0.71 |
| 1:A:141:ARG:O | 1:A:143:THR:HG22 | 1.91 | 0.71 |
| 1:C:141:ARG:O | 1:C:143:THR:HG22 | 1.91 | 0.71 |
| 1:G:90:ARG:NH1 | 1:G:270:SER:O | 2.24 | 0.71 |
| 1:A:106:GLU:CG | 2:B:71:SER:HB2 | 2.09 | 0.70 |
| 1:C:311:HIS:NE2 | 2:D:97:GLU:OE1 | 2.24 | 0.70 |
| 1:G:141:ARG:O | 1:G:143:THR:HG22 | 1.91 | 0.70 |
| 3:J:96:ARG:NH1 | 4:K:47:TRP:CD1 | 2.59 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:101:ARG:HG3 | 5:Q:100:GLY:HA3 | 1.73 | 0.70 |
| 2:B:41:THR:CB | 4:H:100(G):TYR:CZ | 2.75 | 0.70 |
| 1:C:261(G):ILE:CG2 | 5:T:65:SER:O | 2.39 | 0.70 |
| 4:F:56:ALA:HA | 4:F:57:THR:HG22 | 1.74 | 0.70 |
| 1:G:131:ARG:HB2 | 1:G:155:SER:HB2 | 1.72 | 0.70 |
| 1:G:222:LYS:O | 6:U:53:ASN:HB3 | 1.92 | 0.70 |
| 6:R:190:LYS:HE2 | 6:R:210:ASN:HB3 | 1.73 | 0.70 |
| 1:A:221:PRO:HG2 | 6:R:49:TYR:CZ | 2.26 | 0.70 |
| 6:U:190:LYS:HE2 | 6:U:210:ASN:HB3 | 1.73 | 0.70 |
| 2:B:80:LEU:HG | 2:D:80:LEU:HD21 | 1.74 | 0.70 |
| 2:D:54:ARG:NH2 | 2:D:103:GLU:OE2 | 2.24 | 0.69 |
| 3:E:164:THR:HG23 | 4:F:174:PHE:CD2 | 2.28 | 0.69 |
| 6:O:190:LYS:HE2 | 6:O:210:ASN:HB3 | 1.73 | 0.69 |
| 2:B:41:THR:CG2 | 4:H:100(G):TYR:CZ | 2.75 | 0.69 |
| 4:F:11:LEU:HD11 | 4:F:148:PHE:HE2 | 1.54 | 0.69 |
| 1:A:136:THR:HG23 | 1:A:139:CYS:H | 1.58 | 0.69 |
| 1:A:221:PRO:HB2 | 6:R:49:TYR:CD2 | 2.27 | 0.69 |
| 1:C:136:THR:HG23 | 1:C:139:CYS:H | 1.58 | 0.69 |
| 6:O:123:GLU:OE1 | 6:O:123:GLU:N | 2.25 | 0.69 |
| 4:H:56:ALA:HA | 4:H:57:THR:HG22 | 1.74 | 0.69 |
| 4:K:56:ALA:HA | 4:K:57:THR:HG22 | 1.74 | 0.69 |
| 5:Q:212:GLU:OE2 | 5:Q:213:PRO:CD | 2.41 | 0.68 |
| 5:T:212:GLU:OE2 | 5:T:213:PRO:CD | 2.41 | 0.68 |
| 6:R:79:GLN:HG2 | 6:R:80:PRO:HD2 | 1.75 | 0.68 |
| 5:Q:214:LYS:H | 5:Q:214:LYS:CD | 2.00 | 0.68 |
| 5:T:167:PRO:HG2 | 6:U:163:VAL:O | 1.94 | 0.68 |
| 1:A:261(F):GLY:HA2 | 5:N:59:TYR:HE2 | 1.59 | 0.68 |
| 2:B:54:ARG:NH2 | 2:B:103:GLU:OE2 | 2.24 | 0.68 |
| 5:N:212:GLU:OE2 | 5:N:213:PRO:CD | 2.42 | 0.68 |
| 1:G:219:ALA:HB3 | 5:T:1:GLN:OE1 | 1.95 | 0.67 |
| 4:K:114:ALA:HB1 | 4:K:148:PHE:CD2 | 2.28 | 0.67 |
| 4:F:114:ALA:HB1 | 4:F:148:PHE:CD2 | 2.28 | 0.67 |
| 5:N:195:ILE:HG12 | 5:N:195:ILE:O | 1.94 | 0.67 |
| 4:H:114:ALA:HB1 | 4:H:148:PHE:CD2 | 2.28 | 0.67 |
| 2:D:41:THR:HB | 4:F:100(G):TYR:CE2 | 2.30 | 0.67 |
| 1:G:58:ALA:HB1 | 1:G:86:LEU:HD13 | 1.76 | 0.67 |
| 1:G:136:THR:HG23 | 1:G:139:CYS:H | 1.58 | 0.67 |
| 1:A:51:ILE:HG23 | 1:A:282:PHE:CD1 | 2.29 | 0.67 |
| 6:R:190:LYS:NZ | 6:R:190:LYS:C | 2.48 | 0.67 |
| 5:T:166:PHE:CE1 | 6:U:174:SER:C | 2.65 | 0.67 |
| 1:G:219:ALA:CB | 5:T:1:GLN:HE22 | 2.08 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 6:U:190:LYS:NZ | 6:U:190:LYS:C | 2.48 | 0.67 |
| 3:J:202:SER:HB3 | 6:R:173:TYR:OH | 1.95 | 0.67 |
| 2:I:54:ARG:NH2 | 2:I:103:GLU:OE2 | 2.24 | 0.67 |
| 1:C:51:ILE:HG23 | 1:C:282:PHE:CD1 | 2.29 | 0.67 |
| 1:C:101:ARG:HH21 | 5:N:100:GLY:HA2 | 1.60 | 0.66 |
| 6:O:190:LYS:NZ | 6:O:190:LYS:C | 2.48 | 0.66 |
| 1:A:200:LYS:HA | 1:A:248:ASN:ND2 | 2.11 | 0.66 |
| 1:G:51:ILE:HG23 | 1:G:282:PHE:CD1 | 2.30 | 0.66 |
| 1:G:200:LYS:HA | 1:G:248:ASN:ND2 | 2.11 | 0.66 |
| 4:K:112:SER:OG | 4:K:114:ALA:N | 2.29 | 0.66 |
| 5:Q:60:ASN:O | 5:Q:64:LYS:HG3 | 1.94 | 0.66 |
| 5:Q:195:ILE:HG12 | 5:Q:195:ILE:O | 1.94 | 0.66 |
| 6:R:123:GLU:OE1 | 6:R:123:GLU:N | 2.25 | 0.66 |
| 1:C:96:ILE:HD13 | 1:C:99:PRO:HA | 1.78 | 0.66 |
| 1:A:33:ARG:NH1 | 3:J:2:ILE:HD12 | 2.11 | 0.66 |
| 1:A:96:ILE:HD13 | 1:A:99:PRO:HA | 1.78 | 0.66 |
| 3:L:78:LEU:HD11 | 3:L:104:LEU:HD21 | 1.78 | 0.66 |
| 1:G:221:PRO:HB2 | 6:U:49:TYR:CD2 | 2.30 | 0.66 |
| 4:K:28:THR:HG21 | 4:K:94:LYS:HZ1 | 1.61 | 0.66 |
| 5:T:195:ILE:HG12 | 5:T:195:ILE:O | 1.94 | 0.66 |
| 2:D:41:THR:CG2 | 4:F:100(G):TYR:CE1 | 2.75 | 0.65 |
| 1:G:101:ARG:NH2 | 5:T:99:LEU:HD12 | 2.11 | 0.65 |
| 4:H:112:SER:OG | 4:H:114:ALA:N | 2.29 | 0.65 |
| 5:T:105:GLN:HG2 | 6:U:43:ALA:H | 1.62 | 0.65 |
| 1:A:200:LYS:HA | 1:A:248:ASN:HD21 | 1.61 | 0.65 |
| 1:C:200:LYS:HA | 1:C:248:ASN:ND2 | 2.11 | 0.65 |
| 1:G:200:LYS:HA | 1:G:248:ASN:HD21 | 1.61 | 0.65 |
| 1:A:180:TRP:CE2 | 1:A:233:HIS:HB2 | 2.32 | 0.65 |
| 4:F:11:LEU:HD11 | 4:F:148:PHE:CE2 | 2.32 | 0.65 |
| 1:G:96:ILE:HD13 | 1:G:99:PRO:HA | 1.78 | 0.65 |
| 1:G:180:TRP:CE2 | 1:G:233:HIS:HB2 | 2.32 | 0.65 |
| 3:J:78:LEU:HD11 | 3:J:104:LEU:HD21 | 1.78 | 0.65 |
| 4:K:11:LEU:HD11 | 4:K:148:PHE:CE2 | 2.32 | 0.65 |
| 1:G:50:GLU:OE1 | 1:G:274:ILE:HG12 | 1.96 | 0.65 |
| 5:T:59:TYR:O | 5:T:64:LYS:HD3 | 1.97 | 0.65 |
| 3:L:125:LEU:O | 3:L:183:LYS:HD2 | 1.97 | 0.65 |
| 1:A:202:ILE:HG23 | 1:A:247:PHE:HB3 | 1.80 | 0.64 |
| 1:C:261:ARG:HH12 | 1:C:261(H):GLU:HG3 | 1.60 | 0.64 |
| 1:C:200:LYS:HA | 1:C:248:ASN:HD21 | 1.61 | 0.64 |
| 4:F:112:SER:OG | 4:F:114:ALA:N | 2.29 | 0.64 |
| 5:Q:124:LEU:HB3 | 6:R:118:PHE:CZ | 2.32 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:268:ILE:CB | 1:A:284:PRO:O | 2.35 | 0.64 |
| 1:G:101:ARG:HD3 | 5:T:100:GLY:N | 2.12 | 0.64 |
| 3:J:125:LEU:O | 3:J:183:LYS:HD2 | 1.97 | 0.64 |
| 4:K:28:THR:HG21 | 4:K:94:LYS:NZ | 2.13 | 0.64 |
| 6:O:190:LYS:C | 6:O:190:LYS:HZ2 | 2.01 | 0.64 |
| 1:G:86:LEU:HD21 | 1:G:88:ILE:HG12 | 1.79 | 0.64 |
| 2:B:41:THR:HG21 | 4:H:100(G):TYR:CZ | 2.32 | 0.64 |
| 3:E:96:ARG:NH1 | 4:F:47:TRP:CD1 | 2.66 | 0.64 |
| 5:N:159:LEU:HD22 | 5:N:194:TYR:CD1 | 2.33 | 0.64 |
| 5:Q:205:THR:O | 5:Q:206:LYS:HD3 | 1.98 | 0.64 |
| 5:T:105:GLN:HA | 6:U:43:ALA:HA | 1.78 | 0.64 |
| 5:T:205:THR:O | 5:T:206:LYS:HD3 | 1.98 | 0.64 |
| 1:C:180:TRP:CE2 | 1:C:233:HIS:HB2 | 2.32 | 0.64 |
| 3:E:125:LEU:O | 3:E:183:LYS:HD2 | 1.97 | 0.64 |
| 4:F:28:THR:HG21 | 4:F:94:LYS:NZ | 2.13 | 0.64 |
| 1:C:202:ILE:HG23 | 1:C:247:PHE:HB3 | 1.80 | 0.63 |
| 2:B:41:THR:HB | 4:H:100(G):TYR:CE2 | 2.33 | 0.63 |
| 3:E:78:LEU:HD11 | 3:E:104:LEU:HD21 | 1.78 | 0.63 |
| 1:G:261:ARG:HH12 | 1:G:261(H):GLU:HG3 | 1.60 | 0.63 |
| 5:Q:84:ALA:O | 5:Q:87:THR:HG22 | 1.98 | 0.63 |
| 5:T:166:PHE:CE1 | 6:U:174:SER:HB2 | 2.33 | 0.63 |
| 5:T:61:PRO:HA | 5:T:64:LYS:CE | 2.23 | 0.63 |
| 6:U:190:LYS:NZ | 6:U:210:ASN:HA | 2.13 | 0.63 |
| 5:Q:159:LEU:HD22 | 5:Q:194:TYR:CD1 | 2.33 | 0.63 |
| 4:H:28:THR:HG21 | 4:H:94:LYS:NZ | 2.13 | 0.63 |
| 1:G:49:GLY:CA | 1:G:272:ALA:HB3 | 2.23 | 0.63 |
| 6:R:18:ARG:HH21 | 6:R:76:ARG:NH2 | 1.97 | 0.63 |
| 5:T:84:ALA:O | 5:T:87:THR:HG22 | 1.98 | 0.63 |
| 5:T:166:PHE:CZ | 6:U:174:SER:HB2 | 2.33 | 0.63 |
| 6:U:18:ARG:HH21 | 6:U:76:ARG:NH2 | 1.97 | 0.63 |
| 6:U:123:GLU:OE1 | 6:U:123:GLU:N | 2.25 | 0.63 |
| 1:A:261:ARG:HH12 | 1:A:261(H):GLU:HG3 | 1.60 | 0.62 |
| 1:C:173:LYS:CE | 5:T:55:GLY:HA3 | 2.24 | 0.62 |
| 3:L:37:GLN:HB2 | 3:L:47:LEU:HD11 | 1.81 | 0.62 |
| 1:G:202:ILE:HG23 | 1:G:247:PHE:HB3 | 1.80 | 0.62 |
| 5:N:84:ALA:O | 5:N:87:THR:HG22 | 1.98 | 0.62 |
| 5:T:159:LEU:HD22 | 5:T:194:TYR:CD1 | 2.33 | 0.62 |
| 5:Q:169:VAL:HG11 | 6:R:162:SER:HB2 | 1.77 | 0.62 |
| 3:J:199:GLN:HB3 | 6:R:10:SER:OG | 1.99 | 0.62 |
| 6:U:190:LYS:C | 6:U:190:LYS:HZ2 | 2.01 | 0.62 |
| 2:I:56:ILE:HG13 | 4:K:100:ILE:HG12 | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:O:18:ARG:HH21 | 6:O:76:ARG:NH2 | 1.97 | 0.62 |
| 1:C:58:ALA:HB2 | 1:C:86:LEU:HD23 | 1.82 | 0.62 |
| 6:R:190:LYS:NZ | 6:R:210:ASN:HA | 2.13 | 0.62 |
| 1:A:220:ARG:HG2 | 5:Q:96:THR:CG2 | 2.30 | 0.62 |
| 1:A:101:ARG:CG | 5:Q:100:GLY:HA3 | 2.30 | 0.62 |
| 1:A:170:ASN:ND2 | 1:A:237:LEU:O | 2.32 | 0.62 |
| 2:D:38:LEU:HD21 | 4:F:53:ASN:CB | 2.30 | 0.62 |
| 1:A:120:LYS:HB2 | 1:A:256:ARG:HH21 | 1.65 | 0.61 |
| 4:K:13:GLN:HE22 | 4:K:113:SER:CB | 2.13 | 0.61 |
| 3:J:37:GLN:HB2 | 3:J:47:LEU:HD11 | 1.81 | 0.61 |
| 5:Q:212:GLU:CG | 5:Q:213:PRO:CD | 2.76 | 0.61 |
| 5:T:105:GLN:HG2 | 6:U:43:ALA:N | 2.14 | 0.61 |
| 1:A:106:GLU:HB3 | 2:B:71:SER:HB2 | 0.66 | 0.61 |
| 1:C:101:ARG:HH21 | 5:N:100:GLY:CA | 2.13 | 0.61 |
| 1:G:101:ARG:HG2 | 1:G:101:ARG:HH11 | 1.64 | 0.61 |
| 5:T:60:ASN:O | 5:T:64:LYS:HG3 | 2.00 | 0.61 |
| 3:E:37:GLN:HB2 | 3:E:47:LEU:HD11 | 1.81 | 0.61 |
| 5:Q:166:PHE:HE1 | 6:R:174:SER:C | 2.04 | 0.61 |
| 1:G:120:LYS:HB2 | 1:G:256:ARG:HH21 | 1.65 | 0.61 |
| 1:G:170:ASN:ND2 | 1:G:237:LEU:O | 2.32 | 0.61 |
| 6:O:190:LYS:NZ | 6:O:210:ASN:HA | 2.14 | 0.61 |
| 5:T:166:PHE:CE1 | 6:U:174:SER:CB | 2.84 | 0.61 |
| 1:A:33:ARG:HH12 | 3:J:2:ILE:CD1 | 2.14 | 0.61 |
| 4:H:13:GLN:HE22 | 4:H:113:SER:CB | 2.14 | 0.61 |
| 4:H:100(A):TYR:CE1 | 4:H:100(K):TYR:CE2 | 2.88 | 0.61 |
| 1:C:101:ARG:HH21 | 5:N:100:GLY:C | 2.04 | 0.61 |
| 2:I:41:THR:HG21 | 4:K:100(G):TYR:CZ | 2.36 | 0.61 |
| 4:F:13:GLN:HE22 | 4:F:113:SER:CB | 2.14 | 0.60 |
| 1:A:58:ALA:HB2 | 1:A:86:LEU:CD2 | 2.31 | 0.60 |
| 1:A:160:VAL:HA | 1:A:196:GLY:HA3 | 1.83 | 0.60 |
| 1:C:100:GLY:HA3 | 1:C:230:ILE:O | 2.01 | 0.60 |
| 1:C:160:VAL:HA | 1:C:196:GLY:HA3 | 1.83 | 0.60 |
| 1:G:15:LEU:CD1 | 2:I:118:LEU:HG | 2.31 | 0.60 |
| 1:C:170:ASN:ND2 | 1:C:237:LEU:O | 2.32 | 0.60 |
| 1:G:100:GLY:HA3 | 1:G:230:ILE:O | 2.01 | 0.60 |
| 2:B:19:ASP:OD1 | 2:B:19:ASP:N | 2.35 | 0.60 |
| 3:J:94:TRP:HZ3 | 4:K:59:TYR:O | 1.84 | 0.60 |
| 1:A:261(D):PRO:O | 1:A:261(E):SER:HB2 | 2.02 | 0.60 |
| 1:G:172:ARG:HD3 | 1:G:259:PHE:CZ | 2.37 | 0.60 |
| 1:G:261(D):PRO:O | 1:G:261(E):SER:HB2 | 2.02 | 0.60 |
| 1:A:33:ARG:HH22 | 3:J:2:ILE:HD11 | 1.57 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:C:261(D):PRO:O | 1:C:261(E):SER:HB2 | 2.02 | 0.60 |
| 1:A:100:GLY:HA3 | 1:A:230:ILE:O | 2.01 | 0.60 |
| 1:C:172:ARG:HD3 | 1:C:259:PHE:CZ | 2.37 | 0.60 |
| 5:T:137:ALA:CB | 6:U:116:PHE:CZ | 2.85 | 0.60 |
| 1:A:172:ARG:HD3 | 1:A:259:PHE:CZ | 2.37 | 0.60 |
| 1:A:221:PRO:HB2 | 6:R:49:TYR:CZ | 2.34 | 0.60 |
| 1:C:120:LYS:HB2 | 1:C:256:ARG:HH21 | 1.65 | 0.60 |
| 2:D:38:LEU:HD23 | 4:F:53:ASN:HB3 | 1.82 | 0.60 |
| 1:G:130:ILE:HG23 | 1:G:155:SER:O | 2.02 | 0.60 |
| 5:T:137:ALA:HB3 | 6:U:116:PHE:CZ | 2.35 | 0.60 |
| 2:D:124:LYS:HD3 | 2:I:134:GLY:HA2 | 1.84 | 0.60 |
| 1:G:97:CYS:O | 1:G:224:ASN:ND2 | 2.35 | 0.60 |
| 1:G:261(G):ILE:CG2 | 5:Q:65:SER:O | 2.49 | 0.60 |
| 2:I:19:ASP:OD1 | 2:I:19:ASP:N | 2.34 | 0.60 |
| 3:L:124:GLN:HA | 4:H:122:PHE:CE1 | 2.37 | 0.60 |
| 5:T:6:GLU:HG3 | 5:T:92:CYS:SG | 2.42 | 0.60 |
| 4:H:114:ALA:HB1 | 4:H:148:PHE:CE2 | 2.36 | 0.59 |
| 1:A:130:ILE:HG23 | 1:A:155:SER:O | 2.02 | 0.59 |
| 1:G:268:ILE:CG2 | 1:G:284:PRO:HA | 2.31 | 0.59 |
| 5:Q:210:ARG:HG3 | 5:Q:210:ARG:HH11 | 1.67 | 0.59 |
| 2:B:38:LEU:CD2 | 4:H:53:ASN:CB | 2.75 | 0.59 |
| 1:G:160:VAL:HA | 1:G:196:GLY:HA3 | 1.83 | 0.59 |
| 5:N:212:GLU:CG | 5:N:213:PRO:CD | 2.76 | 0.59 |
| 1:A:221:PRO:CB | 6:R:49:TYR:CZ | 2.86 | 0.59 |
| 1:A:261(F):GLY:HA2 | 5:N:59:TYR:CE2 | 2.37 | 0.59 |
| 2:B:38:LEU:HA | 4:H:100(G):TYR:CZ | 2.36 | 0.59 |
| 2:D:41:THR:HB | 4:F:100(G):TYR:CZ | 2.37 | 0.59 |
| 1:A:52:CYS:O | 1:A:56:LYS:HG2 | 2.03 | 0.59 |
| 3:L:96:ARG:NH1 | 4:H:47:TRP:CD1 | 2.71 | 0.59 |
| 1:G:219:ALA:HB1 | 5:T:1:GLN:HE22 | 1.66 | 0.59 |
| 1:C:50:GLU:OE1 | 1:C:274:ILE:HG12 | 2.03 | 0.59 |
| 5:N:18:LEU:HD13 | 5:N:109:VAL:HG11 | 1.85 | 0.59 |
| 5:Q:6:GLU:HG3 | 5:Q:92:CYS:SG | 2.42 | 0.59 |
| 5:Q:143:LYS:HE3 | 6:R:131:SER:OG | 2.01 | 0.59 |
| 1:A:70:ILE:HG21 | 1:A:179:VAL:HG21 | 1.85 | 0.59 |
| 1:A:97:CYS:O | 1:A:224:ASN:ND2 | 2.34 | 0.59 |
| 5:N:6:GLU:HG3 | 5:N:92:CYS:SG | 2.42 | 0.59 |
| 5:N:210:ARG:HG3 | 5:N:210:ARG:HH11 | 1.67 | 0.59 |
| 5:Q:18:LEU:HD13 | 5:Q:109:VAL:HG11 | 1.84 | 0.59 |
| 1:C:97:CYS:O | 1:C:224:ASN:ND2 | 2.35 | 0.58 |
| 1:C:130:ILE:HG23 | 1:C:155:SER:O | 2.02 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:G:15:LEU:HD12 | 2:I:118:LEU:HG | 1.85 | 0.58 |
| 2:I:41:THR:HG21 | 4:K:100(G):TYR:CE1 | 2.38 | 0.58 |
| 1:C:261(G):ILE:HG22 | 5:T:65:SER:O | 2.02 | 0.58 |
| 4:F:28:THR:HG21 | 4:F:94:LYS:HZ1 | 1.68 | 0.58 |
| 5:N:199:ASN:OD1 | 5:N:206:LYS:HG3 | 2.03 | 0.58 |
| 6:R:190:LYS:C | 6:R:190:LYS:HZ2 | 2.05 | 0.58 |
| 5:Q:153:SER:HB2 | 5:Q:197:ASN:HD21 | 1.67 | 0.58 |
| 5:T:210:ARG:HG3 | 5:T:210:ARG:HH11 | 1.67 | 0.58 |
| 1:C:101:ARG:HE | 5:N:100:GLY:HA3 | 1.60 | 0.58 |
| 5:T:18:LEU:HD13 | 5:T:109:VAL:HG11 | 1.85 | 0.58 |
| 1:C:70:ILE:HG21 | 1:C:179:VAL:HG21 | 1.85 | 0.58 |
| 3:E:27:GLN:OE1 | 1:G:33:ARG:CZ | 2.52 | 0.58 |
| 1:G:70:ILE:HG21 | 1:G:179:VAL:HG21 | 1.85 | 0.58 |
| 6:O:143:GLU:O | 6:O:198:HIS:HD2 | 1.87 | 0.58 |
| 6:R:143:GLU:O | 6:R:198:HIS:HD2 | 1.87 | 0.58 |
| 5:T:214:LYS:HD3 | 5:T:214:LYS:N | 2.10 | 0.58 |
| 6:U:143:GLU:O | 6:U:198:HIS:HD2 | 1.87 | 0.58 |
| 1:G:261(E):SER:CB | 5:Q:64:LYS:HE2 | 2.34 | 0.58 |
| 1:G:86:LEU:HD21 | 1:G:88:ILE:CG1 | 2.33 | 0.58 |
| 1:G:101:ARG:CZ | 5:T:99:LEU:HB2 | 2.33 | 0.58 |
| 1:G:261(E):SER:HB3 | 5:Q:64:LYS:HB3 | 1.85 | 0.58 |
| 1:C:50:GLU:HG2 | 1:C:275:ASP:O | 2.03 | 0.57 |
| 3:E:2:ILE:HD12 | 1:G:33:ARG:CZ | 2.33 | 0.57 |
| 1:A:261(C):ALA:HB3 | 1:A:261(I):TYR:HB2 | 1.87 | 0.57 |
| 3:L:164:THR:HG23 | 4:H:174:PHE:CD2 | 2.39 | 0.57 |
| 5:T:153:SER:HB2 | 5:T:197:ASN:HD21 | 1.67 | 0.57 |
| 4:H:114:ALA:CB | 4:H:148:PHE:CD2 | 2.87 | 0.57 |
| 1:C:261(C):ALA:HB3 | 1:C:261(I):TYR:HB2 | 1.87 | 0.57 |
| 4:H:70:SER:HB3 | 4:H:79:TYR:HB2 | 1.86 | 0.57 |
| 4:F:70:SER:HB3 | 4:F:79:TYR:HB2 | 1.86 | 0.57 |
| 4:F:100(H):TYR:CE2 | 4:F:100(J):THR:HA | 2.40 | 0.57 |
| 3:L:202:SER:OG | 6:O:142:ARG:CB | 2.53 | 0.57 |
| 3:J:202:SER:CB | 6:R:173:TYR:OH | 2.51 | 0.57 |
| 4:K:70:SER:HB3 | 4:K:79:TYR:HB2 | 1.86 | 0.57 |
| 5:T:124:LEU:CB | 6:U:118:PHE:CE1 | 2.77 | 0.57 |
| 1:A:103:THR:HG22 | 1:A:233:HIS:HA | 1.87 | 0.57 |
| 4:H:100(H):TYR:CE2 | 4:H:100(J):THR:HA | 2.40 | 0.57 |
| 4:F:114:ALA:CB | 4:F:148:PHE:CD2 | 2.86 | 0.57 |
| 5:N:152:VAL:HG22 | 5:N:198:VAL:HG22 | 1.87 | 0.56 |
| 1:A:206:SER:HB3 | 1:A:209:TYR:HB3 | 1.87 | 0.56 |
| 6:O:103:LYS:NZ | 6:O:165:GLU:OE2 | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 5:T:61:PRO:CB | 5:T:64:LYS:HE2 | 2.35 | 0.56 |
| 5:T:212:GLU:CG | 5:T:213:PRO:CD | 2.76 | 0.56 |
| 1:A:14:CYS:O | 2:B:24:PHE:HA | 2.05 | 0.56 |
| 5:Q:60:ASN:C | 5:Q:64:LYS:HG3 | 2.26 | 0.56 |
| 5:T:105:GLN:HA | 6:U:43:ALA:CA | 2.35 | 0.56 |
| 1:A:221:PRO:CB | 6:R:49:TYR:CD2 | 2.88 | 0.56 |
| 2:B:38:LEU:C | 4:H:100(G):TYR:HE2 | 2.09 | 0.56 |
| 1:C:206:SER:HB3 | 1:C:209:TYR:HB3 | 1.87 | 0.56 |
| 1:C:261(G):ILE:O | 1:C:261(G):ILE:HD12 | 2.06 | 0.56 |
| 1:G:261(G):ILE:HD12 | 1:G:261(G):ILE:O | 2.06 | 0.56 |
| 5:T:60:ASN:C | 5:T:64:LYS:HG3 | 2.26 | 0.56 |
| 3:E:2:ILE:HD12 | 1:G:33:ARG:NH1 | 2.20 | 0.56 |
| 3:E:94:TRP:HZ3 | 4:F:59:TYR:O | 1.87 | 0.56 |
| 1:G:103:THR:HG22 | 1:G:233:HIS:HA | 1.87 | 0.56 |
| 1:C:103:THR:HG22 | 1:C:233:HIS:HA | 1.87 | 0.56 |
| 1:G:261(C):ALA:HB3 | 1:G:261(I):TYR:HB2 | 1.86 | 0.56 |
| 5:Q:142:VAL:HG22 | 5:Q:198:VAL:HG21 | 1.88 | 0.56 |
| 5:Q:152:VAL:HG22 | 5:Q:198:VAL:HG22 | 1.87 | 0.56 |
| 2:D:41:THR:CB | 4:F:100(G):TYR:CZ | 2.88 | 0.56 |
| 1:G:51:ILE:CD1 | 1:G:268:ILE:HD13 | 2.36 | 0.56 |
| 4:K:100(H):TYR:CE2 | 4:K:100(J):THR:HA | 2.40 | 0.56 |
| 1:A:51:ILE:CD1 | 1:A:266:LEU:HD23 | 2.36 | 0.55 |
| 4:F:114:ALA:HB3 | 4:F:148:PHE:HE2 | 1.68 | 0.55 |
| 1:A:261(G):ILE:HG22 | 5:N:64:LYS:O | 2.06 | 0.55 |
| 1:C:58:ALA:HB2 | 1:C:86:LEU:CD2 | 2.36 | 0.55 |
| 5:T:152:VAL:HG22 | 5:T:198:VAL:HG22 | 1.87 | 0.55 |
| 2:B:53:ASN:HB2 | 4:H:100(K):TYR:CZ | 2.40 | 0.55 |
| 5:N:142:VAL:HG22 | 5:N:198:VAL:HG21 | 1.88 | 0.55 |
| 3:E:2:ILE:HD12 | 1:G:33:ARG:HH12 | 1.71 | 0.55 |
| 1:G:206:SER:HB3 | 1:G:209:TYR:HB3 | 1.87 | 0.55 |
| 4:F:4:LEU:HD23 | 4:F:94:LYS:HE2 | 1.89 | 0.55 |
| 4:K:4:LEU:HD23 | 4:K:94:LYS:HE2 | 1.89 | 0.55 |
| 4:K:114:ALA:HB1 | 4:K:148:PHE:CE2 | 2.37 | 0.55 |
| 5:T:142:VAL:HG22 | 5:T:198:VAL:HG21 | 1.87 | 0.55 |
| 1:A:58:ALA:HB2 | 1:A:86:LEU:HD23 | 1.88 | 0.55 |
| 1:A:261(G):ILE:HD12 | 1:A:261(G):ILE:O | 2.06 | 0.55 |
| 1:A:52:CYS:O | 1:A:282:PHE:CE1 | 2.60 | 0.54 |
| 1:G:52:CYS:O | 1:G:282:PHE:CE1 | 2.60 | 0.54 |
| 6:U:103:LYS:NZ | 6:U:165:GLU:OE2 | 2.38 | 0.54 |
| 4:H:4:LEU:HD23 | 4:H:94:LYS:HE2 | 1.89 | 0.54 |
| 4:F:87:THR:HG23 | 4:F:110:THR:HA | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:204:VAL:O | 1:A:210:GLN:HA | 2.08 | 0.54 |
| 2:D:38:LEU:O | 4:F:100(G):TYR:HE2 | 1.89 | 0.54 |
| 1:G:67:LEU:N | 1:G:95:ASP:OD1 | 2.41 | 0.54 |
| 1:G:139:CYS:HB2 | 1:G:146:SER:O | 2.07 | 0.54 |
| 6:R:121:SER:O | 6:R:125:LEU:HD13 | 2.08 | 0.54 |
| 1:C:52:CYS:O | 1:C:282:PHE:CE1 | 2.60 | 0.54 |
| 3:E:105:GLU:CD | 3:E:173:TYR:HH | 2.11 | 0.54 |
| 5:N:153:SER:HB2 | 5:N:197:ASN:HD21 | 1.67 | 0.54 |
| 6:O:121:SER:O | 6:O:125:LEU:HD13 | 2.08 | 0.54 |
| 5:T:166:PHE:HE1 | 6:U:174:SER:O | 1.90 | 0.54 |
| 1:A:139:CYS:HB2 | 1:A:146:SER:O | 2.07 | 0.54 |
| 1:C:204:VAL:O | 1:C:210:GLN:HA | 2.08 | 0.54 |
| 1:G:204:VAL:O | 1:G:210:GLN:HA | 2.08 | 0.54 |
| 5:T:164:HIS:NE2 | 6:U:138:ASN:OD1 | 2.41 | 0.54 |
| 3:L:202:SER:OG | 6:O:142:ARG:HB2 | 2.07 | 0.54 |
| 2:D:19:ASP:OD1 | 2:D:19:ASP:N | 2.35 | 0.54 |
| 3:E:164:THR:HG23 | 4:F:174:PHE:CE2 | 2.42 | 0.54 |
| 4:H:87:THR:HG23 | 4:H:110:THR:HA | 1.89 | 0.53 |
| 1:C:221:PRO:HG2 | 6:O:49:TYR:CE1 | 2.42 | 0.53 |
| 1:A:14:CYS:N | 2:B:25:ARG:O | 2.28 | 0.53 |
| 2:D:38:LEU:HA | 4:F:100(G):TYR:CE2 | 2.43 | 0.53 |
| 5:Q:166:PHE:HZ | 6:R:174:SER:HB3 | 1.73 | 0.53 |
| 1:C:51:ILE:CG1 | 1:C:86:LEU:HD13 | 2.38 | 0.53 |
| 1:C:139:CYS:HB2 | 1:C:146:SER:O | 2.07 | 0.53 |
| 5:Q:163:VAL:HG22 | 5:Q:182:VAL:CG1 | 2.38 | 0.53 |
| 1:C:61:LEU:HB3 | 1:C:64:CYS:HB3 | 1.90 | 0.53 |
| 2:I:42:GLN:NE2 | 4:K:100(H):TYR:O | 2.42 | 0.53 |
| 5:N:163:VAL:HG22 | 5:N:182:VAL:CG1 | 2.38 | 0.53 |
| 6:U:121:SER:O | 6:U:125:LEU:HD13 | 2.08 | 0.53 |
| 1:A:61:LEU:HB3 | 1:A:64:CYS:HB3 | 1.89 | 0.53 |
| 1:A:120:LYS:HB2 | 1:A:256:ARG:NH2 | 2.24 | 0.53 |
| 3:L:48:ILE:HA | 3:L:54:ARG:HA | 1.91 | 0.53 |
| 3:E:48:ILE:HA | 3:E:54:ARG:HA | 1.91 | 0.53 |
| 1:G:61:LEU:HB3 | 1:G:64:CYS:HB3 | 1.89 | 0.53 |
| 3:E:30:ARG:H | 3:E:91:TYR:HE1 | 1.57 | 0.53 |
| 1:G:222:LYS:CE | 1:G:225:GLY:HA2 | 2.39 | 0.53 |
| 2:I:42:GLN:OE1 | 4:K:100(G):TYR:CD2 | 2.62 | 0.53 |
| 4:K:112:SER:OG | 4:K:113:SER:N | 2.42 | 0.53 |
| 4:H:112:SER:OG | 4:H:113:SER:N | 2.42 | 0.53 |
| 6:R:103:LYS:NZ | 6:R:165:GLU:OE2 | 2.38 | 0.53 |
| 3:L:164:THR:HG23 | 4:H:174:PHE:CE2 | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:C:88:ILE:HD12 | 1:C:274:ILE:HD11 | 1.90 | 0.53 |
| 2:I:38:LEU:HD21 | 4:K:53:ASN:HB3 | 1.90 | 0.53 |
| 4:K:87:THR:HG23 | 4:K:110:THR:HA | 1.90 | 0.53 |
| 5:Q:59:TYR:O | 5:Q:64:LYS:HD2 | 2.09 | 0.53 |
| 1:A:67:LEU:N | 1:A:95:ASP:OD1 | 2.41 | 0.53 |
| 3:L:124:GLN:CA | 4:H:122:PHE:CE1 | 2.92 | 0.53 |
| 4:F:51:ILE:HG23 | 4:F:71:ARG:HH21 | 1.74 | 0.53 |
| 5:Q:210:ARG:HG3 | 5:Q:210:ARG:NH1 | 2.24 | 0.53 |
| 1:C:120:LYS:HB2 | 1:C:256:ARG:NH2 | 2.24 | 0.53 |
| 1:G:173:LYS:HE2 | 5:Q:55:GLY:HA3 | 1.90 | 0.53 |
| 5:T:163:VAL:HG22 | 5:T:182:VAL:CG1 | 2.38 | 0.53 |
| 4:H:51:ILE:HG23 | 4:H:71:ARG:HH21 | 1.74 | 0.52 |
| 1:G:88:ILE:HD12 | 1:G:274:ILE:HD11 | 1.90 | 0.52 |
| 3:J:48:ILE:HA | 3:J:54:ARG:HA | 1.91 | 0.52 |
| 5:T:163:VAL:HG22 | 5:T:182:VAL:HG12 | 1.92 | 0.52 |
| 5:T:210:ARG:HG3 | 5:T:210:ARG:NH1 | 2.24 | 0.52 |
| 5:N:210:ARG:HG3 | 5:N:210:ARG:NH1 | 2.24 | 0.52 |
| 5:T:159:LEU:CD2 | 5:T:194:TYR:CE1 | 2.90 | 0.52 |
| 1:A:221:PRO:CG | 6:R:49:TYR:CZ | 2.92 | 0.52 |
| 1:G:120:LYS:HB2 | 1:G:256:ARG:NH2 | 2.24 | 0.52 |
| 1:C:192:ASN:HA | 1:C:196:GLY:O | 2.10 | 0.52 |
| 4:F:112:SER:OG | 4:F:113:SER:N | 2.42 | 0.52 |
| 5:Q:100(A):TYR:C | 6:R:32:PHE:CE2 | 2.83 | 0.52 |
| 3:L:124:GLN:HG3 | 4:H:122:PHE:CZ | 2.45 | 0.52 |
| 1:G:50:GLU:OE1 | 1:G:50:GLU:HA | 2.09 | 0.52 |
| 1:A:91:ARG:NH2 | 1:A:271:ASP:OD2 | 2.43 | 0.52 |
| 1:A:113:ARG:HB3 | 1:A:267:GLY:HA3 | 1.92 | 0.52 |
| 1:G:91:ARG:NH2 | 1:G:271:ASP:OD2 | 2.43 | 0.52 |
| 4:K:51:ILE:HG23 | 4:K:71:ARG:HH21 | 1.74 | 0.52 |
| 1:A:192:ASN:HA | 1:A:196:GLY:O | 2.10 | 0.52 |
| 1:C:261(G):ILE:HG21 | 5:T:65:SER:O | 2.10 | 0.52 |
| 1:G:219:ALA:CB | 5:T:1:GLN:NE2 | 2.72 | 0.52 |
| 5:N:47:TRP:CH2 | 5:N:49:GLY:HA2 | 2.44 | 0.52 |
| 5:T:47:TRP:CH2 | 5:T:49:GLY:HA2 | 2.44 | 0.52 |
| 4:F:100(H):TYR:HE2 | 4:F:100(J):THR:HA | 1.75 | 0.52 |
| 5:N:163:VAL:HG22 | 5:N:182:VAL:HG12 | 1.92 | 0.52 |
| 1:A:88:ILE:HD12 | 1:A:274:ILE:HD11 | 1.90 | 0.52 |
| 3:L:30:ARG:H | 3:L:91:TYR:HE1 | 1.57 | 0.52 |
| 3:J:39:LYS:HG3 | 3:J:84:ALA:HB2 | 1.92 | 0.52 |
| 5:Q:47:TRP:CH2 | 5:Q:49:GLY:HA2 | 2.44 | 0.52 |
| 1:C:91:ARG:NH2 | 1:C:271:ASP:OD2 | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:K:100(H):TYR:HE2 | 4:K:100(J):THR:HA | 1.75 | 0.51 |
| 1:A:268:ILE:CG2 | 1:A:284:PRO:HA | 2.28 | 0.51 |
| 1:C:52:CYS:C | 1:C:56:LYS:HB2 | 2.30 | 0.51 |
| 3:E:105:GLU:CD | 3:E:173:TYR:OH | 2.49 | 0.51 |
| 5:T:47:TRP:CD2 | 6:U:96:PRO:HD2 | 2.45 | 0.51 |
| 5:T:47:TRP:CE3 | 6:U:96:PRO:HD2 | 2.45 | 0.51 |
| 4:H:136:GLY:HA2 | 6:O:156:SER:HB3 | 1.92 | 0.51 |
| 1:C:222:LYS:CE | 1:C:225:GLY:HA2 | 2.39 | 0.51 |
| 1:A:261(G):ILE:CG2 | 5:N:64:LYS:O | 2.59 | 0.51 |
| 3:J:30:ARG:H | 3:J:91:TYR:HE1 | 1.57 | 0.51 |
| 5:Q:163:VAL:HG22 | 5:Q:182:VAL:HG12 | 1.92 | 0.51 |
| 1:C:221:PRO:CG | 6:O:49:TYR:CZ | 2.92 | 0.51 |
| 1:G:113:ARG:HB3 | 1:G:267:GLY:HA3 | 1.92 | 0.51 |
| 1:G:192:ASN:HA | 1:G:196:GLY:O | 2.10 | 0.51 |
| 3:J:105:GLU:CD | 3:J:173:TYR:OH | 2.49 | 0.51 |
| 5:N:154:TRP:CH2 | 5:N:196:CYS:HB3 | 2.46 | 0.51 |
| 6:R:18:ARG:HE | 6:R:76:ARG:NH1 | 2.09 | 0.51 |
| 1:A:181:GLY:HA3 | 1:A:252:ILE:HB | 1.93 | 0.51 |
| 4:F:13:GLN:OE1 | 4:F:113:SER:HA | 2.11 | 0.51 |
| 5:Q:154:TRP:O | 5:Q:155:ASN:CB | 2.35 | 0.51 |
| 5:T:154:TRP:CH2 | 5:T:196:CYS:HB3 | 2.46 | 0.51 |
| 1:A:48:ILE:HD12 | 1:A:50:GLU:OE1 | 2.11 | 0.51 |
| 3:E:39:LYS:HG3 | 3:E:84:ALA:HB2 | 1.93 | 0.51 |
| 3:J:54:ARG:HB2 | 3:J:58:ILE:HD11 | 1.93 | 0.51 |
| 1:C:113:ARG:HB3 | 1:C:267:GLY:HA3 | 1.92 | 0.51 |
| 3:E:2:ILE:CD1 | 1:G:33:ARG:HH12 | 2.24 | 0.51 |
| 3:L:94:TRP:HZ3 | 4:H:59:TYR:O | 1.93 | 0.50 |
| 2:I:38:LEU:CD2 | 4:K:53:ASN:HB3 | 2.41 | 0.50 |
| 4:K:13:GLN:OE1 | 4:K:113:SER:HA | 2.11 | 0.50 |
| 6:O:18:ARG:HE | 6:O:76:ARG:NH1 | 2.09 | 0.50 |
| 5:Q:154:TRP:CH2 | 5:Q:196:CYS:HB3 | 2.46 | 0.50 |
| 4:H:13:GLN:OE1 | 4:H:113:SER:HA | 2.11 | 0.50 |
| 1:G:139:CYS:O | 1:G:146:SER:HB3 | 2.11 | 0.50 |
| 6:U:18:ARG:HE | 6:U:76:ARG:NH1 | 2.09 | 0.50 |
| 3:L:105:GLU:CD | 3:L:173:TYR:OH | 2.49 | 0.50 |
| 1:C:52:CYS:O | 1:C:56:LYS:HG2 | 2.10 | 0.50 |
| 1:G:106:GLU:HB3 | 2:I:71:SER:OG | 2.09 | 0.50 |
| 3:L:213:GLU:O | 3:L:214:CYS:SG | 2.70 | 0.50 |
| 4:H:100(A):TYR:CD1 | 4:H:100(K):TYR:CE2 | 2.98 | 0.50 |
| 2:D:38:LEU:HA | 4:F:100(G):TYR:OH | 2.12 | 0.50 |
| 3:E:213:GLU:O | 3:E:214:CYS:SG | 2.70 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:R:143:GLU:O | 6:R:198:HIS:CD2 | 2.65 | 0.50 |
| 6:U:186:TYR:O | 6:U:192:TYR:OH | 2.30 | 0.50 |
| 3:L:39:LYS:HG3 | 3:L:84:ALA:HB2 | 1.92 | 0.50 |
| 1:C:139:CYS:O | 1:C:146:SER:HB3 | 2.11 | 0.50 |
| 6:O:186:TYR:O | 6:O:192:TYR:OH | 2.30 | 0.50 |
| 1:A:139:CYS:O | 1:A:146:SER:HB3 | 2.11 | 0.50 |
| 1:G:101:ARG:NE | 5:T:99:LEU:HB2 | 2.27 | 0.50 |
| 4:H:100(H):TYR:HE2 | 4:H:100(J):THR:HA | 1.75 | 0.50 |
| 4:H:136:GLY:HA3 | 6:O:156:SER:HB2 | 1.94 | 0.50 |
| 4:F:114:ALA:CB | 4:F:148:PHE:CZ | 2.95 | 0.50 |
| 4:F:59:TYR:CE1 | 4:F:69:ILE:HD13 | 2.47 | 0.50 |
| 4:K:59:TYR:CE1 | 4:K:69:ILE:HD13 | 2.47 | 0.50 |
| 3:L:199:GLN:HG3 | 6:O:10:SER:OG | 2.11 | 0.49 |
| 1:G:14:CYS:O | 2:I:24:PHE:HA | 2.11 | 0.49 |
| 1:G:181:GLY:HA3 | 1:G:252:ILE:HB | 1.93 | 0.49 |
| 6:O:143:GLU:O | 6:O:198:HIS:CD2 | 2.65 | 0.49 |
| 3:L:54:ARG:HB2 | 3:L:58:ILE:HD11 | 1.93 | 0.49 |
| 4:H:213:LYS:N | 4:H:214:PRO:CD | 2.76 | 0.49 |
| 1:C:67:LEU:N | 1:C:95:ASP:OD1 | 2.41 | 0.49 |
| 4:K:13:GLN:HE22 | 4:K:113:SER:HB2 | 1.77 | 0.49 |
| 6:R:186:TYR:O | 6:R:192:TYR:OH | 2.30 | 0.49 |
| 3:E:95:LEU:HG | 4:F:47:TRP:HZ3 | 1.77 | 0.49 |
| 4:K:213:LYS:N | 4:K:214:PRO:CD | 2.75 | 0.49 |
| 5:Q:171:GLN:HA | 6:R:160:GLN:OE1 | 2.12 | 0.49 |
| 6:U:143:GLU:O | 6:U:198:HIS:CD2 | 2.65 | 0.49 |
| 3:E:96:ARG:NH1 | 4:F:47:TRP:NE1 | 2.60 | 0.49 |
| 3:J:213:GLU:O | 3:J:214:CYS:SG | 2.69 | 0.49 |
| 1:A:153:TRP:HZ2 | 1:A:183:HIS:CE1 | 2.31 | 0.49 |
| 1:C:181:GLY:HA3 | 1:C:252:ILE:HB | 1.93 | 0.49 |
| 3:E:54:ARG:HB2 | 3:E:58:ILE:HD11 | 1.93 | 0.49 |
| 4:H:13:GLN:HE22 | 4:H:113:SER:HB2 | 1.77 | 0.49 |
| 1:C:167:THR:HG22 | 1:C:244:THR:OG1 | 2.13 | 0.49 |
| 6:U:103:LYS:CE | 6:U:165:GLU:OE2 | 2.61 | 0.49 |
| 2:B:41:THR:HB | 4:H:100(G):TYR:OH | 2.13 | 0.49 |
| 3:L:33:LEU:HD12 | 3:L:51:ALA:HA | 1.95 | 0.49 |
| 3:L:124:GLN:HG3 | 4:H:122:PHE:CE2 | 2.48 | 0.49 |
| 4:F:213:LYS:N | 4:F:214:PRO:CD | 2.76 | 0.49 |
| 6:R:103:LYS:CE | 6:R:165:GLU:OE2 | 2.61 | 0.49 |
| 1:A:167:THR:HG22 | 1:A:244:THR:OG1 | 2.13 | 0.49 |
| 4:H:59:TYR:CE1 | 4:H:69:ILE:HD13 | 2.47 | 0.49 |
| 1:C:153:TRP:HZ2 | 1:C:183:HIS:CE1 | 2.31 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:K:114:ALA:CB | 4:K:148:PHE:CZ | 2.95 | 0.49 |
| 1:A:222:LYS:CE | 1:A:225:GLY:HA2 | 2.39 | 0.49 |
| 1:A:51:ILE:HB | 1:A:86:LEU:CD2 | 2.32 | 0.48 |
| 1:G:51:ILE:HD13 | 1:G:266:LEU:HD23 | 1.94 | 0.48 |
| 1:G:167:THR:HG22 | 1:G:244:THR:OG1 | 2.13 | 0.48 |
| 1:G:324:PRO:O | 1:G:325:GLU:HB2 | 2.13 | 0.48 |
| 4:H:147:TYR:CE2 | 4:H:152:VAL:HG13 | 2.48 | 0.48 |
| 4:F:187:LEU:C | 4:F:187:LEU:HD12 | 2.34 | 0.48 |
| 5:Q:200:HIS:HB3 | 5:Q:205:THR:OG1 | 2.13 | 0.48 |
| 5:T:208:ASP:C | 5:T:209:LYS:HD2 | 2.33 | 0.48 |
| 1:A:261(E):SER:O | 5:N:59:TYR:HD2 | 1.92 | 0.48 |
| 4:F:147:TYR:CE2 | 4:F:152:VAL:HG13 | 2.48 | 0.48 |
| 5:N:200:HIS:HB3 | 5:N:205:THR:OG1 | 2.13 | 0.48 |
| 5:Q:208:ASP:C | 5:Q:209:LYS:HD2 | 2.32 | 0.48 |
| 5:N:208:ASP:C | 5:N:209:LYS:HD2 | 2.32 | 0.48 |
| 6:O:103:LYS:CE | 6:O:165:GLU:OE2 | 2.61 | 0.48 |
| 4:H:187:LEU:C | 4:H:187:LEU:HD12 | 2.34 | 0.48 |
| 3:J:105:GLU:CD | 3:J:173:TYR:HH | 2.17 | 0.48 |
| 5:N:50:TYR:CE2 | 5:N:58:ASN:HB3 | 2.49 | 0.48 |
| 3:E:33:LEU:HD12 | 3:E:51:ALA:HA | 1.94 | 0.48 |
| 4:F:13:GLN:HE22 | 4:F:113:SER:HB2 | 1.77 | 0.48 |
| 5:Q:43:LYS:HE2 | 5:Q:43:LYS:HB3 | 1.57 | 0.48 |
| 1:A:33:ARG:NH1 | 3:J:2:ILE:CD1 | 2.75 | 0.48 |
| 1:G:51:ILE:HG23 | 1:G:282:PHE:HD1 | 1.79 | 0.48 |
| 1:G:67:LEU:HB2 | 1:G:95:ASP:OD1 | 2.14 | 0.48 |
| 1:G:153:TRP:HZ2 | 1:G:183:HIS:CE1 | 2.31 | 0.48 |
| 1:G:261(E):SER:HG | 5:Q:64:LYS:HE2 | 1.76 | 0.48 |
| 5:T:166:PHE:HD1 | 6:U:164:THR:HG23 | 1.62 | 0.48 |
| 1:A:70:ILE:HD11 | 1:A:112:ILE:HG13 | 1.96 | 0.48 |
| 1:C:101:ARG:NH2 | 5:N:100:GLY:CA | 2.68 | 0.48 |
| 5:N:126:PRO:HG3 | 5:N:189:LEU:HD22 | 1.96 | 0.48 |
| 5:Q:199:ASN:CG | 5:Q:206:LYS:HD2 | 2.34 | 0.48 |
| 2:B:38:LEU:HA | 4:H:100(G):TYR:CE2 | 2.49 | 0.48 |
| 1:C:67:LEU:HB2 | 1:C:95:ASP:OD1 | 2.14 | 0.48 |
| 1:C:70:ILE:HD11 | 1:C:112:ILE:HG13 | 1.95 | 0.48 |
| 4:K:37:VAL:HG22 | 4:K:47:TRP:HA | 1.96 | 0.48 |
| 5:T:126:PRO:HG3 | 5:T:189:LEU:HD22 | 1.96 | 0.48 |
| 5:T:200:HIS:HB3 | 5:T:205:THR:OG1 | 2.13 | 0.48 |
| 1:A:51:ILE:HD12 | 1:A:86:LEU:HD13 | 1.95 | 0.48 |
| 1:G:101:ARG:HH21 | 5:T:99:LEU:HD12 | 1.78 | 0.48 |
| 2:I:42:GLN:OE1 | 4:K:100(G):TYR:HD2 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 5:T:154:TRP:O | 5:T:155:ASN:C | 2.52 | 0.48 |
| 1:A:324:PRO:O | 1:A:325:GLU:HB2 | 2.13 | 0.47 |
| 1:G:300:ILE:HD11 | 2:I:69:GLU:HG3 | 1.96 | 0.47 |
| 5:Q:154:TRP:O | 5:Q:155:ASN:C | 2.52 | 0.47 |
| 5:Q:166:PHE:CE1 | 6:R:164:THR:CG2 | 2.91 | 0.47 |
| 5:Q:169:VAL:HG13 | 6:R:162:SER:CB | 2.35 | 0.47 |
| 1:A:33:ARG:HH12 | 3:J:2:ILE:HD12 | 1.74 | 0.47 |
| 3:L:95:LEU:HD11 | 4:H:61:ASP:H | 1.79 | 0.47 |
| 2:D:38:LEU:O | 4:F:100(G):TYR:CE2 | 2.68 | 0.47 |
| 1:G:156:SER:O | 1:G:157:SER:OG | 2.23 | 0.47 |
| 4:K:187:LEU:C | 4:K:187:LEU:HD12 | 2.34 | 0.47 |
| 5:Q:166:PHE:HA | 6:R:164:THR:HG22 | 1.96 | 0.47 |
| 5:T:50:TYR:CE2 | 5:T:58:ASN:HB3 | 2.49 | 0.47 |
| 5:T:91:PHE:CE1 | 6:U:44:PRO:HD3 | 2.49 | 0.47 |
| 5:T:199:ASN:CG | 5:T:206:LYS:HD2 | 2.34 | 0.47 |
| 1:C:161:PHE:HB3 | 1:C:248:ASN:O | 2.15 | 0.47 |
| 2:D:38:LEU:HA | 4:F:100(G):TYR:HE2 | 1.79 | 0.47 |
| 2:D:159:HIS:CE1 | 2:D:160:ASN:OD1 | 2.67 | 0.47 |
| 1:A:67:LEU:HG | 1:A:109:ARG:HG2 | 1.97 | 0.47 |
| 1:A:101:ARG:CG | 5:Q:100:GLY:CA | 2.82 | 0.47 |
| 4:H:100(A):TYR:CD1 | 4:H:100(K):TYR:HE2 | 2.31 | 0.47 |
| 1:G:51:ILE:HB | 1:G:86:LEU:HD12 | 1.94 | 0.47 |
| 3:J:199:GLN:CB | 6:R:10:SER:OG | 2.62 | 0.47 |
| 5:Q:61:PRO:HA | 5:Q:64:LYS:HD3 | 1.95 | 0.47 |
| 1:A:222:LYS:O | 6:R:53:ASN:HB3 | 2.13 | 0.47 |
| 1:C:51:ILE:HD12 | 1:C:86:LEU:HB2 | 1.96 | 0.47 |
| 1:C:161:PHE:HA | 1:C:162:PRO:HD3 | 1.74 | 0.47 |
| 1:G:161:PHE:HB3 | 1:G:248:ASN:O | 2.15 | 0.47 |
| 1:A:51:ILE:CB | 1:A:86:LEU:HD22 | 2.32 | 0.47 |
| 1:A:67:LEU:HB2 | 1:A:95:ASP:OD1 | 2.14 | 0.47 |
| 1:A:182:VAL:HG22 | 1:A:202:ILE:HD12 | 1.97 | 0.47 |
| 2:B:53:ASN:OD1 | 2:B:53:ASN:O | 2.33 | 0.47 |
| 2:B:170:ARG:HH21 | 2:I:128:GLU:CD | 2.18 | 0.47 |
| 4:H:100(J):THR:HG23 | 4:H:100(K):TYR:CZ | 2.49 | 0.47 |
| 4:H:114:ALA:HB3 | 4:H:148:PHE:HE2 | 1.68 | 0.47 |
| 1:C:324:PRO:O | 1:C:325:GLU:HB2 | 2.13 | 0.47 |
| 1:G:70:ILE:HD11 | 1:G:112:ILE:HG13 | 1.95 | 0.47 |
| 2:I:159:HIS:CE1 | 2:I:160:ASN:OD1 | 2.67 | 0.47 |
| 4:K:115:SER:O | 4:K:116:THR:C | 2.52 | 0.47 |
| 4:K:147:TYR:CE2 | 4:K:152:VAL:HG13 | 2.48 | 0.47 |
| 5:N:154:TRP:O | 5:N:155:ASN:C | 2.52 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:T:137:ALA:HB3 | 6:U:116:PHE:CE1 | 2.50 | 0.47 |
| 4:H:37:VAL:HG22 | 4:H:47:TRP:HA | 1.96 | 0.47 |
| 3:J:33:LEU:HD12 | 3:J:51:ALA:HA | 1.95 | 0.47 |
| 5:Q:50:TYR:CE2 | 5:Q:58:ASN:HB3 | 2.49 | 0.47 |
| 5:Q:124:LEU:HD12 | 6:R:118:PHE:CD2 | 2.50 | 0.47 |
| 3:J:199:GLN:CG | 6:R:10:SER:OG | 2.63 | 0.47 |
| 1:A:71:ILE:HG22 | 1:A:151:MET:HE3 | 1.97 | 0.47 |
| 1:G:71:ILE:HG22 | 1:G:151:MET:HE3 | 1.97 | 0.47 |
| 5:Q:159:LEU:CD2 | 5:Q:194:TYR:CE1 | 2.90 | 0.47 |
| 2:B:159:HIS:CE1 | 2:B:160:ASN:OD1 | 2.68 | 0.46 |
| 4:H:114:ALA:CB | 4:H:148:PHE:CZ | 2.95 | 0.46 |
| 1:C:71:ILE:CG2 | 1:C:151:MET:HE1 | 2.45 | 0.46 |
| 1:C:223:VAL:HG22 | 6:O:53:ASN:ND2 | 2.29 | 0.46 |
| 1:G:67:LEU:HG | 1:G:109:ARG:HG2 | 1.97 | 0.46 |
| 5:T:170:LEU:O | 6:U:160:GLN:NE2 | 2.46 | 0.46 |
| 1:A:180:TRP:NE1 | 1:A:233:HIS:HB2 | 2.31 | 0.46 |
| 5:N:154:TRP:O | 5:N:155:ASN:CB | 2.35 | 0.46 |
| 4:H:115:SER:O | 4:H:116:THR:C | 2.53 | 0.46 |
| 1:G:177:LEU:HB3 | 1:G:258:THR:HB | 1.98 | 0.46 |
| 5:N:159:LEU:CD2 | 5:N:194:TYR:CE1 | 2.90 | 0.46 |
| 5:T:137:ALA:HB2 | 6:U:116:PHE:CZ | 2.49 | 0.46 |
| 1:C:62:GLY:HA2 | 1:C:90:ARG:HG3 | 1.98 | 0.46 |
| 1:C:177:LEU:HB3 | 1:C:258:THR:HB | 1.98 | 0.46 |
| 6:O:67:SER:HA | 6:O:71:PHE:CE2 | 2.51 | 0.46 |
| 5:Q:126:PRO:HG3 | 5:Q:189:LEU:HD22 | 1.96 | 0.46 |
| 1:A:161:PHE:HB3 | 1:A:248:ASN:O | 2.15 | 0.46 |
| 3:L:121:SER:HB3 | 4:H:123:PRO:HD2 | 1.96 | 0.46 |
| 4:H:39:GLN:HB2 | 4:H:45:LEU:HD13 | 1.98 | 0.46 |
| 1:C:67:LEU:HG | 1:C:109:ARG:HG2 | 1.97 | 0.46 |
| 1:G:158(A):ASN:OD1 | 1:G:193:LYS:HE2 | 2.16 | 0.46 |
| 5:T:59:TYR:CB | 5:T:64:LYS:HG2 | 2.37 | 0.46 |
| 3:E:199:GLN:CD | 6:U:10:SER:OG | 2.54 | 0.46 |
| 4:F:37:VAL:HG22 | 4:F:47:TRP:HA | 1.96 | 0.46 |
| 4:F:115:SER:O | 4:F:116:THR:C | 2.52 | 0.46 |
| 1:G:17:HIS:HA | 2:I:21:TRP:O | 2.16 | 0.46 |
| 1:C:71:ILE:HG21 | 1:C:151:MET:HE1 | 1.98 | 0.46 |
| 1:C:156:SER:O | 1:C:157:SER:OG | 2.23 | 0.46 |
| 4:F:145:LYS:HE3 | 4:F:179:GLN:OE1 | 2.16 | 0.46 |
| 1:G:51:ILE:HD12 | 1:G:86:LEU:HG | 1.96 | 0.46 |
| 1:G:62:GLY:HA2 | 1:G:90:ARG:HG3 | 1.98 | 0.46 |
| 2:B:53:ASN:HB2 | 4:H:100(K):TYR:OH | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:L:91:TYR:HB2 | 3:L:92:ASN:HB3 | 1.98 | 0.46 |
| 1:G:182:VAL:HG22 | 1:G:202:ILE:HD12 | 1.97 | 0.46 |
| 4:H:145:LYS:HE3 | 4:H:179:GLN:OE1 | 2.16 | 0.46 |
| 3:E:95:LEU:HD11 | 4:F:61:ASP:H | 1.81 | 0.46 |
| 2:B:38:LEU:HD22 | 4:H:53:ASN:HB3 | 1.93 | 0.45 |
| 1:C:182:VAL:HG22 | 1:C:202:ILE:HD12 | 1.97 | 0.45 |
| 1:G:13:LEU:CD2 | 2:I:152:ILE:HG21 | 2.45 | 0.45 |
| 5:Q:166:PHE:CZ | 6:R:174:SER:HB3 | 2.51 | 0.45 |
| 5:T:166:PHE:HZ | 6:U:174:SER:CB | 2.13 | 0.45 |
| 1:A:158(A):ASN:OD1 | 1:A:193:LYS:HE2 | 2.16 | 0.45 |
| 1:A:177:LEU:HB3 | 1:A:258:THR:HB | 1.98 | 0.45 |
| 1:A:300:ILE:HD11 | 2:B:69:GLU:HG3 | 1.98 | 0.45 |
| 1:G:108:LEU:HD13 | 1:G:234:TRP:CE3 | 2.52 | 0.45 |
| 1:A:56:LYS:HD3 | 1:A:56:LYS:HA | 1.76 | 0.45 |
| 1:C:180:TRP:NE1 | 1:C:233:HIS:HB2 | 2.31 | 0.45 |
| 1:C:200:LYS:HD3 | 1:C:248:ASN:ND2 | 2.31 | 0.45 |
| 1:G:13:LEU:HD22 | 2:I:152:ILE:HG21 | 1.98 | 0.45 |
| 1:G:166:GLN:HB2 | 1:G:245:PHE:HB2 | 1.98 | 0.45 |
| 1:G:219:ALA:CB | 5:T:1:GLN:OE1 | 2.64 | 0.45 |
| 3:J:91:TYR:HB2 | 3:J:92:ASN:HB3 | 1.98 | 0.45 |
| 1:A:200:LYS:HA | 1:A:200:LYS:HD3 | 1.78 | 0.45 |
| 1:C:157:SER:O | 1:C:158:MET:HG3 | 2.17 | 0.45 |
| 1:C:173:LYS:HD2 | 1:C:173:LYS:N | 2.32 | 0.45 |
| 3:E:91:TYR:HB2 | 3:E:92:ASN:HB3 | 1.98 | 0.45 |
| 1:G:52:CYS:O | 1:G:282:PHE:HE1 | 2.00 | 0.45 |
| 1:G:157:SER:O | 1:G:158:MET:HG3 | 2.17 | 0.45 |
| 1:G:200:LYS:HD3 | 1:G:248:ASN:ND2 | 2.31 | 0.45 |
| 1:C:108:LEU:HD13 | 1:C:234:TRP:CE3 | 2.52 | 0.45 |
| 1:C:166:GLN:HB2 | 1:C:245:PHE:HB2 | 1.99 | 0.45 |
| 3:J:96:ARG:NH1 | 4:K:100(N):MET:HE3 | 2.32 | 0.45 |
| 5:N:214:LYS:CD | 5:N:214:LYS:N | 2.75 | 0.45 |
| 5:T:91:PHE:CE1 | 6:U:44:PRO:CD | 2.99 | 0.45 |
| 6:U:67:SER:HA | 6:U:71:PHE:CE2 | 2.51 | 0.45 |
| 1:A:33:ARG:HH11 | 3:J:93:HIS:HB2 | 1.81 | 0.45 |
| 1:A:51:ILE:O | 1:A:86:LEU:HD22 | 2.17 | 0.45 |
| 1:A:200:LYS:HD3 | 1:A:248:ASN:ND2 | 2.31 | 0.45 |
| 3:E:12:SER:HA | 3:E:105:GLU:HB2 | 1.99 | 0.45 |
| 3:E:95:LEU:HA | 4:F:47:TRP:CZ3 | 2.52 | 0.45 |
| 1:G:180:TRP:NE1 | 1:G:233:HIS:HB2 | 2.31 | 0.45 |
| 1:A:131:ARG:CG | 1:A:157:SER:HA | 2.41 | 0.45 |
| 1:A:157:SER:O | 1:A:158:MET:HG3 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:261(D):PRO:O | 5:N:57:THR:O | 2.35 | 0.45 |
| 1:C:134:GLY:HA3 | 1:C:153:TRP:HB3 | 1.98 | 0.45 |
| 6:R:67:SER:HA | 6:R:71:PHE:CE2 | 2.51 | 0.45 |
| 1:A:108:LEU:HD13 | 1:A:234:TRP:CE3 | 2.52 | 0.45 |
| 1:C:158(A):ASN:OD1 | 1:C:193:LYS:HE2 | 2.16 | 0.45 |
| 4:K:39:GLN:HB2 | 4:K:45:LEU:HD13 | 1.98 | 0.45 |
| 5:Q:166:PHE:CZ | 6:R:174:SER:CB | 3.00 | 0.45 |
| 1:A:48:ILE:H | 1:A:48:ILE:HG13 | 1.55 | 0.45 |
| 2:B:173:ILE:HA | 2:I:164:ASP:OD1 | 2.17 | 0.45 |
| 3:L:124:GLN:HB2 | 4:H:122:PHE:CD1 | 2.52 | 0.45 |
| 4:F:30:ARG:NH2 | 4:F:71:ARG:HG3 | 2.32 | 0.45 |
| 3:J:164:THR:HG23 | 4:K:174:PHE:CE2 | 2.52 | 0.45 |
| 5:Q:105:GLN:HG2 | 6:R:43:ALA:N | 2.32 | 0.45 |
| 1:C:108:LEU:HD13 | 1:C:234:TRP:CD2 | 2.52 | 0.44 |
| 1:A:58:ALA:CB | 1:A:86:LEU:HG | 2.47 | 0.44 |
| 1:A:108:LEU:HD13 | 1:A:234:TRP:CD2 | 2.52 | 0.44 |
| 1:A:172:ARG:HD3 | 1:A:259:PHE:CE2 | 2.52 | 0.44 |
| 1:G:134:GLY:HA3 | 1:G:153:TRP:HB3 | 1.98 | 0.44 |
| 4:K:145:LYS:HE3 | 4:K:179:GLN:OE1 | 2.16 | 0.44 |
| 5:Q:214:LYS:CD | 5:Q:214:LYS:N | 2.75 | 0.44 |
| 1:C:52:CYS:O | 1:C:282:PHE:HE1 | 2.00 | 0.44 |
| 1:C:223:VAL:O | 1:C:224:ASN:HB2 | 2.17 | 0.44 |
| 2:D:38:LEU:CA | 4:F:100(G):TYR:HE2 | 2.30 | 0.44 |
| 1:G:223:VAL:O | 1:G:224:ASN:HB2 | 2.18 | 0.44 |
| 3:L:12:SER:HA | 3:L:105:GLU:HB2 | 1.99 | 0.44 |
| 4:F:39:GLN:HB2 | 4:F:45:LEU:HD13 | 1.98 | 0.44 |
| 1:A:62:GLY:HA2 | 1:A:90:ARG:HG3 | 1.98 | 0.44 |
| 1:A:130:ILE:HG22 | 1:A:131:ARG:O | 2.18 | 0.44 |
| 3:L:199:GLN:CG | 6:O:10:SER:OG | 2.66 | 0.44 |
| 4:H:30:ARG:NH2 | 4:H:71:ARG:HG3 | 2.32 | 0.44 |
| 1:G:130:ILE:HG22 | 1:G:131:ARG:O | 2.18 | 0.44 |
| 1:G:172:ARG:HD3 | 1:G:259:PHE:CE2 | 2.52 | 0.44 |
| 1:G:54:LYS:HD2 | 1:G:276(A):SER:O | 2.18 | 0.44 |
| 1:A:221:PRO:HG2 | 6:R:49:TYR:CE1 | 2.52 | 0.44 |
| 1:A:223:VAL:O | 1:A:224:ASN:HB2 | 2.18 | 0.44 |
| 4:H:100(N):MET:H | 4:H:100(N):MET:HG2 | 1.60 | 0.44 |
| 1:C:54:LYS:HD2 | 1:C:276(A):SER:O | 2.18 | 0.44 |
| 1:C:172:ARG:HD3 | 1:C:259:PHE:CE2 | 2.52 | 0.44 |
| 1:G:173:LYS:HD2 | 1:G:173:LYS:N | 2.32 | 0.44 |
| 1:G:221:PRO:CB | 6:U:49:TYR:CD2 | 3.01 | 0.44 |
| 5:T:123:PRO:HB3 | 5:T:211:VAL:HG13 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:A:134:GLY:HA3 | 1:A:153:TRP:HB3 | 1.98 | 0.44 |
| 1:A:166:GLN:HB2 | 1:A:245:PHE:HB2 | 1.99 | 0.44 |
| 2:B:53:ASN:ND2 | 4:H:100(K):TYR:CE1 | 2.79 | 0.44 |
| 4:H:100(J):THR:HG23 | 4:H:100(K):TYR:CD1 | 2.52 | 0.44 |
| 1:G:221:PRO:HG2 | 6:U:49:TYR:CZ | 2.52 | 0.44 |
| 5:Q:167:PRO:HG2 | 6:R:163:VAL:O | 2.18 | 0.44 |
| 6:U:33:LEU:HD21 | 6:U:88:CYS:HB2 | 2.00 | 0.44 |
| 6:U:48:ILE:HD12 | 6:U:73:LEU:HD13 | 1.99 | 0.44 |
| 3:L:121:SER:CB | 4:H:123:PRO:HD2 | 2.48 | 0.44 |
| 4:H:4:LEU:HD11 | 4:H:92:CYS:O | 2.18 | 0.44 |
| 1:C:82:PHE:CE2 | 1:C:117:GLY:HA2 | 2.53 | 0.44 |
| 1:A:54:LYS:HD2 | 1:A:276(A):SER:O | 2.18 | 0.43 |
| 1:C:51:ILE:HG23 | 1:C:282:PHE:HD1 | 1.79 | 0.43 |
| 1:G:108:LEU:HD13 | 1:G:234:TRP:CD2 | 2.52 | 0.43 |
| 5:N:212:GLU:CD | 5:N:213:PRO:CD | 2.86 | 0.43 |
| 6:O:48:ILE:HD12 | 6:O:73:LEU:HD13 | 1.99 | 0.43 |
| 1:G:82:PHE:CE2 | 1:G:117:GLY:HA2 | 2.53 | 0.43 |
| 5:N:123:PRO:HB3 | 5:N:211:VAL:HG13 | 2.00 | 0.43 |
| 1:A:51:ILE:HG23 | 1:A:282:PHE:HD1 | 1.78 | 0.43 |
| 1:A:82:PHE:CE2 | 1:A:117:GLY:HA2 | 2.53 | 0.43 |
| 1:A:114:GLU:HA | 1:A:265:SER:O | 2.18 | 0.43 |
| 1:A:117:GLY:C | 1:A:261:ARG:HG3 | 2.39 | 0.43 |
| 4:H:11:LEU:HG | 4:H:110:THR:OG1 | 2.18 | 0.43 |
| 1:G:96:ILE:HD11 | 5:T:100(A):TYR:OH | 2.17 | 0.43 |
| 4:K:4:LEU:HD11 | 4:K:92:CYS:O | 2.18 | 0.43 |
| 6:O:33:LEU:HD21 | 6:O:88:CYS:HB2 | 2.00 | 0.43 |
| 6:R:33:LEU:HD21 | 6:R:88:CYS:HB2 | 2.00 | 0.43 |
| 5:T:169:VAL:HG11 | 6:U:161:GLU:O | 2.18 | 0.43 |
| 5:T:212:GLU:CD | 5:T:213:PRO:CD | 2.86 | 0.43 |
| 1:C:67:LEU:HD23 | 1:C:67:LEU:HA | 1.64 | 0.43 |
| 1:C:86:LEU:HG | 1:C:86:LEU:O | 2.19 | 0.43 |
| 1:C:114:GLU:HA | 1:C:265:SER:O | 2.18 | 0.43 |
| 1:C:130:ILE:HG22 | 1:C:131:ARG:O | 2.18 | 0.43 |
| 1:C:221:PRO:HB3 | 6:O:49:TYR:CG | 2.53 | 0.43 |
| 4:F:4:LEU:HD11 | 4:F:92:CYS:O | 2.18 | 0.43 |
| 3:J:16:GLY:H | 3:J:78:LEU:HB3 | 1.84 | 0.43 |
| 5:Q:167:PRO:HD3 | 6:R:164:THR:HA | 2.00 | 0.43 |
| 2:B:80:LEU:HD21 | 2:I:80:LEU:HG | 2.01 | 0.43 |
| 3:J:12:SER:HA | 3:J:105:GLU:HB2 | 1.99 | 0.43 |
| 3:J:47:LEU:HB3 | 3:J:48:ILE:HD12 | 2.00 | 0.43 |
| 6:R:48:ILE:HD12 | 6:R:73:LEU:HD13 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:156:SER:O | 1:A:157:SER:OG | 2.23 | 0.43 |
| 1:C:52:CYS:HA | 1:C:54:LYS:N | 2.34 | 0.43 |
| 3:E:47:LEU:HB3 | 3:E:48:ILE:HD12 | 2.01 | 0.43 |
| 3:E:92:ASN:OD1 | 3:E:92:ASN:N | 2.52 | 0.43 |
| 5:Q:212:GLU:CD | 5:Q:213:PRO:CD | 2.86 | 0.43 |
| 1:G:11:ALA:O | 2:I:140:ILE:HB | 2.18 | 0.43 |
| 3:J:80:SER:HA | 3:J:106:ILE:HG12 | 2.01 | 0.43 |
| 4:K:30:ARG:NH2 | 4:K:71:ARG:HG3 | 2.32 | 0.43 |
| 5:Q:100(A):TYR:O | 6:R:32:PHE:CD2 | 2.71 | 0.43 |
| 2:B:80:LEU:CG | 2:D:80:LEU:HD21 | 2.46 | 0.43 |
| 2:B:134:GLY:HA2 | 2:I:124:LYS:HD3 | 2.00 | 0.43 |
| 3:L:7:SER:HA | 3:L:8:PRO:HA | 1.87 | 0.43 |
| 1:C:117:GLY:C | 1:C:261:ARG:HG3 | 2.39 | 0.43 |
| 4:F:94:LYS:HG3 | 4:F:102:VAL:HB | 2.01 | 0.43 |
| 1:G:101:ARG:HG2 | 1:G:101:ARG:NH1 | 2.32 | 0.43 |
| 1:G:131:ARG:CG | 1:G:157:SER:HA | 2.41 | 0.43 |
| 1:A:16:GLY:HA3 | 2:B:14:TRP:CH2 | 2.54 | 0.43 |
| 1:A:52:CYS:C | 1:A:56:LYS:HG2 | 2.40 | 0.42 |
| 3:L:47:LEU:HB3 | 3:L:48:ILE:HD12 | 2.00 | 0.42 |
| 3:L:185:ASP:HA | 3:L:188:LYS:HD3 | 2.01 | 0.42 |
| 4:H:94:LYS:HG3 | 4:H:102:VAL:HB | 2.01 | 0.42 |
| 1:G:114:GLU:HA | 1:G:265:SER:O | 2.18 | 0.42 |
| 1:A:86:LEU:HG | 1:A:86:LEU:O | 2.20 | 0.42 |
| 1:C:101:ARG:NH1 | 1:C:105:GLU:OE2 | 2.52 | 0.42 |
| 3:E:16:GLY:H | 3:E:78:LEU:HB3 | 1.84 | 0.42 |
| 3:E:131:SER:HG | 4:F:145:LYS:HZ3 | 1.62 | 0.42 |
| 1:G:108:LEU:HD22 | 1:G:234:TRP:CD1 | 2.55 | 0.42 |
| 6:R:125:LEU:HB3 | 6:R:183:LYS:HD2 | 2.01 | 0.42 |
| 6:U:125:LEU:HB3 | 6:U:183:LYS:HD2 | 2.00 | 0.42 |
| 1:A:161:PHE:HA | 1:A:162:PRO:HD3 | 1.74 | 0.42 |
| 4:H:51:ILE:HG21 | 4:H:78:LEU:HD13 | 2.02 | 0.42 |
| 1:C:131:ARG:CG | 1:C:157:SER:HA | 2.41 | 0.42 |
| 4:F:51:ILE:HG21 | 4:F:78:LEU:HD13 | 2.02 | 0.42 |
| 3:J:205:VAL:CG2 | 6:R:143:GLU:OE1 | 2.67 | 0.42 |
| 5:T:78:PHE:CZ | 5:T:92:CYS:HB2 | 2.54 | 0.42 |
| 5:T:124:LEU:C | 6:U:118:PHE:CE1 | 2.93 | 0.42 |
| 1:A:197:THR:HG22 | 1:A:198:GLY:N | 2.35 | 0.42 |
| 1:A:199:ASN:O | 1:A:248:ASN:ND2 | 2.52 | 0.42 |
| 3:L:92:ASN:OD1 | 3:L:92:ASN:N | 2.52 | 0.42 |
| 3:J:92:ASN:OD1 | 3:J:92:ASN:N | 2.52 | 0.42 |
| 4:K:13:GLN:HA | 4:K:112:SER:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:108:LEU:HD22 | 1:A:234:TRP:CD1 | 2.54 | 0.42 |
| 1:C:105:GLU:HG3 | 1:C:106:GLU:OE1 | 2.20 | 0.42 |
| 1:G:117:GLY:C | 1:G:261:ARG:HG3 | 2.39 | 0.42 |
| 1:G:146:SER:OG | 1:G:147:PHE:N | 2.53 | 0.42 |
| 3:J:91:TYR:HA | 3:J:92:ASN:HA | 1.80 | 0.42 |
| 5:N:78:PHE:CZ | 5:N:92:CYS:HB2 | 2.54 | 0.42 |
| 5:T:59:TYR:O | 5:T:64:LYS:CG | 2.68 | 0.42 |
| 5:T:212:GLU:CD | 5:T:213:PRO:HD2 | 2.40 | 0.42 |
| 4:H:14:PRO:HD3 | 4:H:112:SER:C | 2.40 | 0.42 |
| 3:E:185:ASP:HA | 3:E:188:LYS:HD3 | 2.02 | 0.42 |
| 1:G:199:ASN:O | 1:G:248:ASN:ND2 | 2.52 | 0.42 |
| 4:K:114:ALA:HB3 | 4:K:148:PHE:HE2 | 1.68 | 0.42 |
| 5:T:124:LEU:HB3 | 6:U:118:PHE:CD1 | 2.46 | 0.42 |
| 1:A:52:CYS:O | 1:A:282:PHE:HE1 | 2.00 | 0.42 |
| 3:L:80:SER:HA | 3:L:106:ILE:HG12 | 2.01 | 0.42 |
| 4:H:58:TYR:HE2 | 4:H:100(H):TYR:CG | 2.38 | 0.42 |
| 1:C:146:SER:OG | 1:C:147:PHE:N | 2.53 | 0.42 |
| 1:C:197:THR:HG22 | 1:C:198:GLY:N | 2.35 | 0.42 |
| 1:G:11:ALA:O | 2:I:140:ILE:N | 2.38 | 0.42 |
| 1:G:86:LEU:HD22 | 1:G:87:ILE:N | 2.23 | 0.42 |
| 1:A:17:HIS:HA | 2:B:21:TRP:O | 2.20 | 0.42 |
| 1:C:199:ASN:O | 1:C:248:ASN:ND2 | 2.52 | 0.42 |
| 4:K:215:SER:O | 4:K:217:THR:HG23 | 2.20 | 0.42 |
| 1:A:51:ILE:HG13 | 1:A:268:ILE:HD13 | 2.01 | 0.42 |
| 1:A:73:PRO:HD2 | 1:A:76:CYS:HB2 | 2.02 | 0.42 |
| 3:L:61:ARG:HD2 | 3:L:77:SER:O | 2.20 | 0.42 |
| 1:C:50:GLU:CD | 1:C:274:ILE:HG23 | 2.39 | 0.42 |
| 1:C:200:LYS:HA | 1:C:200:LYS:HD3 | 1.77 | 0.42 |
| 3:E:80:SER:HA | 3:E:106:ILE:HG12 | 2.01 | 0.42 |
| 2:I:56:ILE:HG21 | 4:K:100:ILE:HG21 | 2.00 | 0.42 |
| 5:Q:212:GLU:CD | 5:Q:213:PRO:HD2 | 2.39 | 0.42 |
| 1:A:83:LYS:HD3 | 1:A:262:ASN:HB2 | 2.02 | 0.42 |
| 3:E:30:ARG:N | 3:E:91:TYR:HE1 | 2.18 | 0.42 |
| 4:F:215:SER:O | 4:F:217:THR:HG23 | 2.20 | 0.42 |
| 4:K:14:PRO:HD3 | 4:K:112:SER:C | 2.40 | 0.42 |
| 6:O:125:LEU:HB3 | 6:O:183:LYS:HD2 | 2.00 | 0.42 |
| 5:Q:78:PHE:CZ | 5:Q:92:CYS:HB2 | 2.54 | 0.42 |
| 5:Q:123:PRO:HB3 | 5:Q:211:VAL:HG13 | 2.00 | 0.42 |
| 3:L:16:GLY:H | 3:L:78:LEU:HB3 | 1.84 | 0.41 |
| 1:C:108:LEU:HD22 | 1:C:234:TRP:CD1 | 2.55 | 0.41 |
| 4:F:13:GLN:HA | 4:F:112:SER:O | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 4:F:14:PRO:HD3 | 4:F:112:SER:C | 2.40 | 0.41 |
| 3:E:34:ALA:HB3 | 3:E:89:GLN:HG2 | 2.02 | 0.41 |
| 1:G:73:PRO:HD2 | 1:G:76:CYS:HB2 | 2.02 | 0.41 |
| 3:J:61:ARG:HD2 | 3:J:77:SER:O | 2.20 | 0.41 |
| 3:J:185:ASP:HA | 3:J:188:LYS:HD3 | 2.02 | 0.41 |
| 4:K:94:LYS:HG3 | 4:K:102:VAL:HB | 2.01 | 0.41 |
| 1:A:109:ARG:O | 1:A:113:ARG:HG3 | 2.21 | 0.41 |
| 1:A:146:SER:OG | 1:A:147:PHE:N | 2.53 | 0.41 |
| 1:C:52:CYS:O | 1:C:56:LYS:CG | 2.68 | 0.41 |
| 1:C:73:PRO:HD2 | 1:C:76:CYS:HB2 | 2.02 | 0.41 |
| 3:E:61:ARG:HD2 | 3:E:77:SER:O | 2.20 | 0.41 |
| 4:F:58:TYR:HE2 | 4:F:100(H):TYR:CG | 2.38 | 0.41 |
| 1:G:197:THR:HG22 | 1:G:198:GLY:N | 2.35 | 0.41 |
| 1:G:201:LEU:HD11 | 1:G:212:SER:HB2 | 2.03 | 0.41 |
| 5:N:142:VAL:CG2 | 5:N:198:VAL:HG21 | 2.51 | 0.41 |
| 5:Q:100(A):TYR:C | 6:R:32:PHE:HE2 | 2.24 | 0.41 |
| 5:Q:100(G):CYS:SG | 6:R:91:SER:CB | 3.09 | 0.41 |
| 5:T:142:VAL:CG2 | 5:T:198:VAL:HG21 | 2.51 | 0.41 |
| 4:H:13:GLN:HA | 4:H:112:SER:O | 2.19 | 0.41 |
| 1:G:71:ILE:HG21 | 1:G:151:MET:HE1 | 2.03 | 0.41 |
| 5:Q:100(G):CYS:SG | 6:R:91:SER:HB2 | 2.61 | 0.41 |
| 1:A:48:ILE:HB | 1:A:50:GLU:OE1 | 2.20 | 0.41 |
| 2:B:171:PHE:HD1 | 2:I:167:LEU:HD13 | 1.86 | 0.41 |
| 1:C:83:LYS:HD3 | 1:C:262:ASN:HB2 | 2.02 | 0.41 |
| 1:G:83:LYS:HD3 | 1:G:262:ASN:HB2 | 2.02 | 0.41 |
| 5:Q:59:TYR:O | 5:Q:64:LYS:CG | 2.68 | 0.41 |
| 1:C:86:LEU:HD11 | 1:C:88:ILE:HG12 | 2.03 | 0.41 |
| 1:C:261(G):ILE:HG22 | 5:T:65:SER:HA | 2.02 | 0.41 |
| 1:G:161:PHE:HA | 1:G:162:PRO:HD3 | 1.74 | 0.41 |
| 1:A:169:ARG:HB2 | 1:A:242:THR:HG22 | 2.02 | 0.41 |
| 3:L:30:ARG:N | 3:L:91:TYR:HE1 | 2.18 | 0.41 |
| 3:L:105:GLU:CD | 3:L:173:TYR:HH | 2.23 | 0.41 |
| 1:C:221:PRO:HB3 | 6:O:49:TYR:CD2 | 2.55 | 0.41 |
| 3:J:35:TRP:CE3 | 3:J:73:LEU:HD22 | 2.56 | 0.41 |
| 3:J:95:LEU:HA | 4:K:47:TRP:CZ3 | 2.56 | 0.41 |
| 4:K:51:ILE:HG21 | 4:K:78:LEU:HD13 | 2.02 | 0.41 |
| 4:K:58:TYR:HE2 | 4:K:100(H):TYR:CG | 2.38 | 0.41 |
| 5:N:124:LEU:HB3 | 6:O:118:PHE:CD1 | 2.56 | 0.41 |
| 5:Q:142:VAL:CG2 | 5:Q:198:VAL:HG21 | 2.51 | 0.41 |
| 5:Q:214:LYS:HD3 | 5:Q:214:LYS:N | 2.10 | 0.41 |
| 5:T:122:PHE:O | 5:T:141:LEU:N | 2.46 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:E:95:LEU:HG | 4:F:47:TRP:CZ3 | 2.56 | 0.41 |
| 5:T:59:TYR:O | 5:T:64:LYS:CD | 2.67 | 0.41 |
| 3:L:34:ALA:HB3 | 3:L:89:GLN:HG2 | 2.02 | 0.40 |
| 3:J:15:PRO:HA | 3:J:78:LEU:HD22 | 2.03 | 0.40 |
| 5:T:39:GLN:NE2 | 6:U:87:TYR:OH | 2.32 | 0.40 |
| 1:A:107:ALA:N | 2:B:71:SER:OG | 2.54 | 0.40 |
| 1:A:166:GLN:O | 1:A:245:PHE:N | 2.38 | 0.40 |
| 1:A:201:LEU:HD11 | 1:A:212:SER:HB2 | 2.03 | 0.40 |
| 3:L:35:TRP:CE3 | 3:L:73:LEU:HD22 | 2.56 | 0.40 |
| 1:C:34:ILE:HD11 | 1:C:321:ARG:NE | 2.37 | 0.40 |
| 1:C:144:VAL:HG22 | 1:C:145:SER:N | 2.37 | 0.40 |
| 1:C:173:LYS:O | 1:C:239:PRO:HG3 | 2.22 | 0.40 |
| 1:G:15:LEU:HD11 | 2:I:118:LEU:HG | 2.00 | 0.40 |
| 1:G:261(C):ALA:HA | 1:G:261(D):PRO:HD2 | 1.90 | 0.40 |
| 6:O:18:ARG:HH21 | 6:O:76:ARG:CZ | 2.34 | 0.40 |
| 6:U:18:ARG:HH21 | 6:U:76:ARG:CZ | 2.34 | 0.40 |
| 1:A:71:ILE:HG21 | 1:A:151:MET:HE1 | 2.03 | 0.40 |
| 3:L:15:PRO:HA | 3:L:78:LEU:HD22 | 2.03 | 0.40 |
| 1:C:71:ILE:HG22 | 1:C:151:MET:CE | 2.51 | 0.40 |
| 1:C:71:ILE:HG22 | 1:C:151:MET:HE3 | 2.03 | 0.40 |
| 1:C:109:ARG:O | 1:C:113:ARG:HG3 | 2.20 | 0.40 |
| 1:G:34:ILE:HD11 | 1:G:321:ARG:NE | 2.37 | 0.40 |
| 4:H:215:SER:O | 4:H:217:THR:HG23 | 2.20 | 0.40 |
| 1:C:221:PRO:HD2 | 5:N:98:ASP:OD2 | 2.21 | 0.40 |
| 6:R:18:ARG:HH21 | 6:R:76:ARG:CZ | 2.34 | 0.40 |
| 2:B:38:LEU:CA | 4:H:100(G):TYR:CE2 | 3.04 | 0.40 |
| 1:G:173:LYS:O | 1:G:239:PRO:HG3 | 2.22 | 0.40 |
| 5:T:43:LYS:HE2 | 5:T:43:LYS:HB3 | 1.57 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | A | 316/333 (95%) | 307 (97%) | 7 (2%) | 2 (1%) | 25 | 65 |
| 1 | C | 313/333 (94%) | 306 (98%) | 5 (2%) | 2 (1%) | 25 | 65 |
| 1 | G | 316/333 (95%) | 308 (98%) | 6 (2%) | 2 (1%) | 25 | 65 |
| 2 | B | 171/176 (97%) | 164 (96%) | 7 (4%) | 0 | 100 | 100 |
| 2 | D | 168/176 (96%) | 161 (96%) | 7 (4%) | 0 | 100 | 100 |
| 2 | I | 171/176 (97%) | 164 (96%) | 7 (4%) | 0 | 100 | 100 |
| 3 | E | 209/214 (98%) | 193 (92%) | 13 (6%) | 3 (1%) | 11 | 46 |
| 3 | J | 209/214 (98%) | 193 (92%) | 13 (6%) | 3 (1%) | 11 | 46 |
| 3 | L | 209/214 (98%) | 193 (92%) | 13 (6%) | 3 (1%) | 11 | 46 |
| 4 | F | 222/234 (95%) | 209 (94%) | 11 (5%) | 2 (1%) | 17 | 56 |
| 4 | H | 222/234 (95%) | 209 (94%) | 11 (5%) | 2 (1%) | 17 | 56 |
| 4 | K | 222/234 (95%) | 209 (94%) | 11 (5%) | 2 (1%) | 17 | 56 |
| 5 | N | 218/229 (95%) | 209 (96%) | 8 (4%) | 1 (0%) | 29 | 69 |
| 5 | Q | 215/229 (94%) | 208 (97%) | 6 (3%) | 1 (0%) | 29 | 69 |
| 5 | T | 215/229 (94%) | 208 (97%) | 6 (3%) | 1 (0%) | 29 | 69 |
| 6 | O | 211/214 (99%) | 207 (98%) | 4 (2%) | 0 | 100 | 100 |
| 6 | R | 211/214 (99%) | 207 (98%) | 4 (2%) | 0 | 100 | 100 |
| 6 | U | 211/214 (99%) | 207 (98%) | 4 (2%) | 0 | 100 | 100 |
| All | All | 4029/4200 (96%) | 3862 (96%) | 143 (4%) | 24 (1%) | 25 | 65 |

All (24) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | L | 94 | TRP |
| 3 | E | 94 | TRP |
| 3 | J | 94 | TRP |
| 1 | A | 141 | ARG |
| 3 | L | 76 | SER |
| 1 | C | 141 | ARG |
| 3 | E | 76 | SER |
| 1 | G | 141 | ARG |
| 3 | J | 76 | SER |
| 3 | L | 51 | ALA |
| 3 | E | 51 | ALA |
| 3 | J | 51 | ALA |
| 4 | H | 114 | ALA |
| 4 | F | 114 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 4 | K | 114 | ALA |
| 1 | A | 261(G) | ILE |
| 1 | C | 261(G) | ILE |
| 1 | G | 261(G) | ILE |
| 4 | H | 52(A) | GLY |
| 4 | F | 52(A) | GLY |
| 4 | K | 52(A) | GLY |
| 5 | N | 213 | PRO |
| 5 | Q | 213 | PRO |
| 5 | T | 213 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | A | 275/285 (96%) | 269 (98%) | 6 (2%) | 52 | 71 |
| 1 | C | 274/285 (96%) | 268 (98%) | 6 (2%) | 52 | 71 |
| 1 | G | 275/285 (96%) | 269 (98%) | 6 (2%) | 52 | 71 |
| 2 | B | 146/148 (99%) | 144 (99%) | 2 (1%) | 67 | 81 |
| 2 | D | 145/148 (98%) | 143 (99%) | 2 (1%) | 67 | 81 |
| 2 | I | 146/148 (99%) | 144 (99%) | 2 (1%) | 67 | 81 |
| 3 | E | 186/187 (100%) | 182 (98%) | 4 (2%) | 52 | 71 |
| 3 | J | 186/187 (100%) | 182 (98%) | 4 (2%) | 52 | 71 |
| 3 | L | 186/187 (100%) | 182 (98%) | 4 (2%) | 52 | 71 |
| 4 | F | 189/196 (96%) | 182 (96%) | 7 (4%) | 34 | 58 |
| 4 | H | 189/196 (96%) | 182 (96%) | 7 (4%) | 34 | 58 |
| 4 | K | 189/196 (96%) | 181 (96%) | 8 (4%) | 30 | 54 |
| 5 | N | 192/199 (96%) | 182 (95%) | 10 (5%) | 23 | 49 |
| 5 | Q | 192/199 (96%) | 182 (95%) | 10 (5%) | 23 | 49 |
| 5 | T | 191/199 (96%) | 182 (95%) | 9 (5%) | 26 | 52 |
| 6 | O | 189/190 (100%) | 187 (99%) | 2 (1%) | 73 | 85 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 6 | R | 189/190 (100%) | 187 (99%) | 2 (1%) | 73 | 85 |
| 6 | U | 189/190 (100%) | 187 (99%) | 2 (1%) | 73 | 85 |
| All | All | 3528/3615 (98%) | 3435 (97%) | 93 (3%) | 46 | 67 |

All (93) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 18 | HIS |
| 1 | A | 48 | ILE |
| 1 | A | 86 | LEU |
| 1 | A | 137 | SER |
| 1 | A | 158(A) | ASN |
| 1 | A | 264 | LYS |
| 2 | B | 19 | ASP |
| 2 | B | 125 | GLN |
| 3 | L | 29 | VAL |
| 3 | L | 33 | LEU |
| 3 | L | 58 | ILE |
| 3 | L | 90 | GLN |
| 4 | H | 2 | VAL |
| 4 | H | 28 | THR |
| 4 | H | 29 | PHE |
| 4 | H | 57 | THR |
| 4 | H | 100(D) | MET |
| 4 | H | 115 | SER |
| 4 | H | 187 | LEU |
| 1 | C | 18 | HIS |
| 1 | C | 48 | ILE |
| 1 | C | 86 | LEU |
| 1 | C | 137 | SER |
| 1 | C | 158(A) | ASN |
| 1 | C | 264 | LYS |
| 2 | D | 19 | ASP |
| 2 | D | 125 | GLN |
| 3 | E | 29 | VAL |
| 3 | E | 33 | LEU |
| 3 | E | 58 | ILE |
| 3 | E | 90 | GLN |
| 4 | F | 2 | VAL |
| 4 | F | 28 | THR |
| 4 | F | 29 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 4 | F | 57 | THR |
| 4 | F | 100(D) | MET |
| 4 | F | 115 | SER |
| 4 | F | 187 | LEU |
| 1 | G | 18 | HIS |
| 1 | G | 48 | ILE |
| 1 | G | 86 | LEU |
| 1 | G | 137 | SER |
| 1 | G | 158(A) | ASN |
| 1 | G | 264 | LYS |
| 2 | I | 19 | ASP |
| 2 | I | 125 | GLN |
| 3 | J | 29 | VAL |
| 3 | J | 33 | LEU |
| 3 | J | 58 | ILE |
| 3 | J | 90 | GLN |
| 4 | K | 2 | VAL |
| 4 | K | 28 | THR |
| 4 | K | 29 | PHE |
| 4 | K | 57 | THR |
| 4 | K | 100(D) | MET |
| 4 | K | 115 | SER |
| 4 | K | 187 | LEU |
| 4 | K | 216 | ASN |
| 5 | N | 31 | SER |
| 5 | N | 33 | ILE |
| 5 | N | 140 | CYS |
| 5 | N | 156 | SER |
| 5 | N | 192 | GLN |
| 5 | N | 193 | THR |
| 5 | N | 195 | ILE |
| 5 | N | 209 | LYS |
| 5 | N | 211 | VAL |
| 5 | N | 214 | LYS |
| 6 | O | 1 | ASP |
| 6 | O | 135 | LEU |
| 5 | Q | 31 | SER |
| 5 | Q | 33 | ILE |
| 5 | Q | 140 | CYS |
| 5 | Q | 156 | SER |
| 5 | Q | 192 | GLN |
| 5 | Q | 193 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | Q | 195 | ILE |
| 5 | Q | 209 | LYS |
| 5 | Q | 211 | VAL |
| 5 | Q | 214 | LYS |
| 6 | R | 1 | ASP |
| 6 | R | 135 | LEU |
| 5 | T | 31 | SER |
| 5 | T | 33 | ILE |
| 5 | T | 140 | CYS |
| 5 | T | 192 | GLN |
| 5 | T | 193 | THR |
| 5 | T | 195 | ILE |
| 5 | T | 209 | LYS |
| 5 | T | 211 | VAL |
| 5 | T | 214 | LYS |
| 6 | U | 1 | ASP |
| 6 | U | 135 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 42 | GLN |
| 2 | B | 159 | HIS |
| 3 | L | 32 | ASN |
| 3 | L | 147 | GLN |
| 3 | L | 210 | ASN |
| 4 | H | 13 | GLN |
| 2 | D | 159 | HIS |
| 3 | E | 147 | GLN |
| 3 | E | 210 | ASN |
| 4 | F | 13 | GLN |
| 2 | I | 159 | HIS |
| 3 | J | 147 | GLN |
| 3 | J | 210 | ASN |
| 4 | K | 13 | GLN |
| 4 | K | 172 | HIS |
| 4 | K | 211 | ASN |
| 6 | O | 199 | GLN |
| 6 | R | 138 | ASN |
| 6 | R | 199 | GLN |
| 5 | T | 39 | GLN |
| 6 | U | 199 | GLN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 322/333 (96%) | 1.22 | 69 (21%) 0 2 | 219, 365, 393, 401 | 0 |
| 1 | C | 321/333 (96%) | 1.13 | 62 (19%) 1 2 | 219, 348, 383, 391 | 0 |
| 1 | G | 322/333 (96%) | 1.39 | 72 (22%) 0 2 | 219, 375, 402, 405 | 0 |
| 2 | B | 173/176 (98%) | 0.66 | 9 (5%) 27 25 | 213, 245, 324, 353 | 0 |
| 2 | D | 172/176 (97%) | 0.71 | 11 (6%) 19 17 | 214, 248, 328, 355 | 0 |
| 2 | I | 173/176 (98%) | 0.68 | 11 (6%) 19 17 | 215, 248, 325, 359 | 0 |
| 3 | E | 213/214 (99%) | 0.66 | 26 (12%) 4 7 | 246, 298, 321, 344 | 0 |
| 3 | J | 213/214 (99%) | 0.64 | 13 (6%) 21 19 | 244, 289, 328, 366 | 0 |
| 3 | L | 213/214 (99%) | 0.49 | 14 (6%) 18 16 | 245, 279, 309, 331 | 0 |
| 4 | F | 226/234 (96%) | 0.77 | 27 (11%) 4 7 | 230, 276, 345, 359 | 0 |
| 4 | H | 226/234 (96%) | 0.61 | 15 (6%) 18 16 | 239, 268, 306, 315 | 0 |
| 4 | K | 226/234 (96%) | 0.68 | 21 (9%) 8 10 | 228, 267, 327, 340 | 0 |
| 5 | N | 222/229 (96%) | 0.98 | 45 (20%) 1 2 | 303, 333, 349, 359 | 0 |
| 5 | Q | 221/229 (96%) | 1.02 | 44 (19%) 1 2 | 328, 347, 373, 381 | 0 |
| 5 | T | 221/229 (96%) | 1.34 | 59 (26%) 0 1 | 337, 370, 384, 388 | 0 |
| 6 | O | 213/214 (99%) | 0.81 | 24 (11%) 5 7 | 287, 309, 343, 348 | 0 |
| 6 | R | 213/214 (99%) | 1.13 | 44 (20%) 1 2 | 330, 347, 366, 372 | 0 |
| 6 | U | 213/214 (99%) | 1.09 | 45 (21%) 1 2 | 336, 357, 385, 388 | 0 |
| All | All | 4103/4200 (97%) | 0.92 | 611 (14%) 2 4 | 213, 317, 386, 405 | 0 |

All (611) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | G | 51 | ILE | 13.2 |
| 1 | A | 181 | GLY | 11.1 |
| 1 | A | 182 | VAL | 10.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | C | 51 | ILE | 9.7 |
| 1 | G | 59 | VAL | 8.7 |
| 1 | A | 250 | ALA | 8.6 |
| 1 | C | 251 | PHE | 8.6 |
| 1 | A | 252 | ILE | 8.3 |
| 1 | G | 120 | LYS | 8.2 |
| 4 | K | 127 | SER | 8.2 |
| 5 | T | 194 | TYR | 8.1 |
| 5 | T | 211 | VAL | 7.9 |
| 1 | G | 250 | ALA | 7.7 |
| 1 | G | 60 | ASP | 7.7 |
| 1 | C | 261(E) | SER | 7.5 |
| 4 | K | 225 | VAL | 7.3 |
| 1 | C | 250 | ALA | 7.2 |
| 1 | C | 261(F) | GLY | 7.1 |
| 1 | G | 127 | TYR | 7.0 |
| 2 | B | 65 | GLN | 6.6 |
| 1 | G | 58 | ALA | 6.6 |
| 1 | C | 49 | GLY | 6.5 |
| 1 | C | 50 | GLU | 6.4 |
| 5 | T | 118 | GLY | 6.4 |
| 5 | Q | 143 | LYS | 6.4 |
| 1 | A | 70 | ILE | 6.4 |
| 1 | C | 214 | SER | 6.3 |
| 5 | T | 1 | GLN | 6.3 |
| 1 | G | 179 | VAL | 6.2 |
| 5 | Q | 120 | SER | 6.2 |
| 1 | G | 252 | ILE | 6.1 |
| 1 | G | 251 | PHE | 6.1 |
| 4 | K | 126 | PRO | 6.1 |
| 1 | G | 181 | GLY | 6.1 |
| 5 | N | 138 | LEU | 6.1 |
| 1 | G | 261(F) | GLY | 6.1 |
| 5 | Q | 121 | VAL | 6.0 |
| 5 | T | 100(E) | GLY | 6.0 |
| 1 | C | 261(D) | PRO | 5.9 |
| 5 | T | 119 | PRO | 5.9 |
| 1 | G | 86 | LEU | 5.9 |
| 1 | A | 251 | PHE | 5.9 |
| 1 | C | 121 | GLU | 5.9 |
| 1 | G | 254 | PRO | 5.8 |
| 5 | Q | 119 | PRO | 5.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | A | 127 | TYR | 5.7 |
| 5 | N | 137 | ALA | 5.7 |
| 3 | L | 37 | GLN | 5.6 |
| 5 | Q | 123 | PRO | 5.6 |
| 1 | G | 88 | ILE | 5.6 |
| 3 | E | 37 | GLN | 5.5 |
| 5 | T | 27 | VAL | 5.5 |
| 1 | A | 214 | SER | 5.5 |
| 1 | G | 50 | GLU | 5.4 |
| 1 | C | 154 | LEU | 5.4 |
| 1 | G | 182 | VAL | 5.4 |
| 1 | G | 183 | HIS | 5.4 |
| 6 | R | 96 | PRO | 5.4 |
| 5 | T | 8 | GLY | 5.3 |
| 1 | A | 51 | ILE | 5.2 |
| 5 | Q | 100(H) | PRO | 5.2 |
| 1 | A | 128 | SER | 5.1 |
| 1 | A | 132 | THR | 5.1 |
| 4 | F | 36 | TRP | 5.1 |
| 1 | G | 154 | LEU | 5.0 |
| 6 | R | 181 | LEU | 5.0 |
| 5 | T | 100(F) | SER | 5.0 |
| 2 | D | 68 | LYS | 5.0 |
| 1 | G | 121 | GLU | 5.0 |
| 1 | A | 274 | ILE | 4.9 |
| 5 | N | 51 | ILE | 4.9 |
| 6 | O | 63 | SER | 4.9 |
| 1 | A | 71 | ILE | 4.9 |
| 6 | U | 146 | VAL | 4.8 |
| 2 | I | 68 | LYS | 4.8 |
| 4 | K | 222 | ARG | 4.8 |
| 1 | G | 132 | THR | 4.7 |
| 1 | G | 52 | CYS | 4.7 |
| 1 | A | 261(H) | GLU | 4.6 |
| 5 | T | 213 | PRO | 4.6 |
| 1 | C | 254 | PRO | 4.6 |
| 1 | G | 256 | ARG | 4.6 |
| 5 | N | 126 | PRO | 4.6 |
| 6 | R | 2 | ILE | 4.5 |
| 1 | C | 166 | GLN | 4.5 |
| 5 | T | 2 | VAL | 4.5 |
| 1 | C | 181 | GLY | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | G | 46 | SER | 4.5 |
| 5 | N | 143 | LYS | 4.5 |
| 3 | E | 98 | PHE | 4.4 |
| 5 | T | 127 | SER | 4.4 |
| 5 | Q | 94 | ARG | 4.4 |
| 6 | U | 155 | GLN | 4.4 |
| 1 | C | 247 | PHE | 4.4 |
| 5 | T | 210 | ARG | 4.4 |
| 5 | T | 184 | VAL | 4.4 |
| 6 | O | 62 | PHE | 4.3 |
| 5 | T | 183 | THR | 4.3 |
| 1 | A | 261(F) | GLY | 4.3 |
| 6 | U | 106 | ILE | 4.3 |
| 5 | T | 35(A) | TRP | 4.3 |
| 1 | G | 217 | PRO | 4.3 |
| 1 | A | 230 | ILE | 4.3 |
| 1 | A | 249 | GLY | 4.3 |
| 6 | R | 145 | LYS | 4.3 |
| 6 | R | 146 | VAL | 4.3 |
| 6 | R | 134 | CYS | 4.2 |
| 5 | N | 71 | ILE | 4.2 |
| 1 | G | 70 | ILE | 4.2 |
| 1 | C | 213 | PHE | 4.2 |
| 1 | A | 235 | MET | 4.1 |
| 1 | G | 87 | ILE | 4.1 |
| 5 | Q | 183 | THR | 4.1 |
| 1 | C | 195 | TYR | 4.1 |
| 5 | T | 48 | ILE | 4.1 |
| 4 | F | 226 | GLU | 4.1 |
| 1 | A | 243 | VAL | 4.1 |
| 3 | E | 119 | PRO | 4.0 |
| 3 | L | 212 | GLY | 4.0 |
| 2 | I | 70 | PHE | 4.0 |
| 4 | F | 227 | PRO | 4.0 |
| 1 | C | 249 | GLY | 4.0 |
| 3 | J | 98 | PHE | 4.0 |
| 5 | Q | 122 | PHE | 4.0 |
| 4 | H | 94 | LYS | 3.9 |
| 5 | N | 140 | CYS | 3.9 |
| 5 | T | 29 | VAL | 3.9 |
| 6 | O | 36 | PHE | 3.9 |
| 1 | C | 153 | TRP | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | G | 61 | LEU | 3.9 |
| 4 | K | 221 | LYS | 3.9 |
| 1 | A | 69 | THR | 3.9 |
| 1 | C | 261(H) | GLU | 3.9 |
| 5 | Q | 184 | VAL | 3.9 |
| 6 | O | 35 | TRP | 3.9 |
| 6 | U | 144 | ALA | 3.9 |
| 1 | G | 163 | GLN | 3.9 |
| 2 | B | 64 | HIS | 3.9 |
| 2 | D | 143 | LYS | 3.9 |
| 1 | A | 154 | LEU | 3.9 |
| 4 | F | 162 | ASN | 3.9 |
| 1 | C | 58 | ALA | 3.8 |
| 5 | T | 71 | ILE | 3.8 |
| 1 | G | 235 | MET | 3.8 |
| 6 | U | 196 | VAL | 3.8 |
| 1 | G | 261(D) | PRO | 3.8 |
| 1 | C | 202 | ILE | 3.8 |
| 4 | F | 37 | VAL | 3.8 |
| 4 | F | 228 | LYS | 3.8 |
| 1 | G | 261(E) | SER | 3.8 |
| 4 | F | 206 | TYR | 3.8 |
| 5 | N | 50 | TYR | 3.8 |
| 5 | T | 214 | LYS | 3.8 |
| 6 | O | 150 | VAL | 3.8 |
| 5 | N | 183 | THR | 3.7 |
| 6 | U | 35 | TRP | 3.7 |
| 5 | N | 179 | SER | 3.7 |
| 1 | C | 245 | PHE | 3.7 |
| 3 | J | 36 | TYR | 3.7 |
| 2 | B | 70 | PHE | 3.7 |
| 1 | C | 232 | PHE | 3.7 |
| 3 | E | 120 | PRO | 3.7 |
| 1 | A | 254 | PRO | 3.7 |
| 6 | R | 130 | ALA | 3.7 |
| 5 | T | 100(D) | SER | 3.7 |
| 1 | A | 183 | HIS | 3.7 |
| 4 | K | 206 | TYR | 3.7 |
| 1 | C | 160 | VAL | 3.7 |
| 5 | Q | 142 | VAL | 3.7 |
| 3 | L | 45 | ARG | 3.7 |
| 5 | Q | 101 | ASN | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | A | 61 | LEU | 3.7 |
| 5 | N | 142 | VAL | 3.7 |
| 1 | C | 182 | VAL | 3.6 |
| 1 | A | 231 | ASP | 3.6 |
| 1 | C | 87 | ILE | 3.6 |
| 5 | T | 70 | SER | 3.6 |
| 2 | D | 69 | GLU | 3.6 |
| 1 | C | 261(G) | ILE | 3.6 |
| 1 | G | 261(H) | GLU | 3.6 |
| 5 | Q | 213 | PRO | 3.6 |
| 1 | A | 46 | SER | 3.6 |
| 1 | A | 47 | SER | 3.6 |
| 1 | A | 273 | GLN | 3.6 |
| 5 | T | 181 | VAL | 3.6 |
| 5 | N | 182 | VAL | 3.6 |
| 4 | F | 35 | SER | 3.6 |
| 1 | A | 213 | PHE | 3.5 |
| 1 | C | 127 | TYR | 3.5 |
| 3 | L | 214 | CYS | 3.5 |
| 5 | N | 213 | PRO | 3.5 |
| 5 | T | 185 | PRO | 3.5 |
| 5 | Q | 144 | ASP | 3.5 |
| 1 | G | 62 | GLY | 3.5 |
| 6 | U | 36 | PHE | 3.5 |
| 4 | H | 200 | THR | 3.5 |
| 6 | R | 97 | THR | 3.5 |
| 6 | O | 64 | GLY | 3.5 |
| 6 | R | 131 | SER | 3.5 |
| 6 | U | 145 | LYS | 3.5 |
| 1 | C | 253 | ALA | 3.4 |
| 5 | Q | 35(A) | TRP | 3.4 |
| 1 | A | 167 | THR | 3.4 |
| 3 | E | 194 | CYS | 3.4 |
| 4 | F | 94 | LYS | 3.4 |
| 1 | G | 122 | SER | 3.4 |
| 4 | F | 166 | LEU | 3.4 |
| 4 | F | 127 | SER | 3.4 |
| 3 | L | 98 | PHE | 3.4 |
| 5 | Q | 127 | SER | 3.4 |
| 4 | K | 140 | LEU | 3.4 |
| 1 | C | 59 | VAL | 3.4 |
| 1 | C | 246 | THR | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | C | 201 | LEU | 3.4 |
| 5 | T | 47 | TRP | 3.4 |
| 1 | A | 195 | TYR | 3.3 |
| 2 | B | 66 | ILE | 3.3 |
| 4 | F | 126 | PRO | 3.3 |
| 6 | R | 62 | PHE | 3.3 |
| 3 | J | 47 | LEU | 3.3 |
| 6 | R | 12 | SER | 3.3 |
| 6 | U | 132 | VAL | 3.3 |
| 1 | A | 261(E) | SER | 3.3 |
| 1 | A | 268 | ILE | 3.3 |
| 1 | C | 191 | GLN | 3.3 |
| 1 | G | 159 | GLN | 3.3 |
| 5 | N | 139 | GLY | 3.3 |
| 3 | E | 34 | ALA | 3.3 |
| 5 | T | 35(B) | THR | 3.3 |
| 6 | U | 133 | VAL | 3.3 |
| 6 | U | 210 | ASN | 3.3 |
| 3 | E | 84 | ALA | 3.3 |
| 6 | U | 207 | LYS | 3.3 |
| 1 | G | 71 | ILE | 3.3 |
| 1 | C | 71 | ILE | 3.3 |
| 1 | G | 191 | GLN | 3.3 |
| 5 | N | 123 | PRO | 3.3 |
| 4 | K | 125 | ALA | 3.3 |
| 4 | F | 196 | SER | 3.3 |
| 1 | G | 89 | GLU | 3.2 |
| 2 | I | 67 | GLU | 3.2 |
| 3 | E | 193 | ALA | 3.2 |
| 6 | U | 89 | GLN | 3.2 |
| 5 | T | 3 | GLN | 3.2 |
| 1 | A | 253 | ALA | 3.2 |
| 5 | N | 212 | GLU | 3.2 |
| 6 | O | 106 | ILE | 3.2 |
| 5 | Q | 141 | LEU | 3.2 |
| 1 | G | 236 | LEU | 3.2 |
| 1 | C | 215 | PRO | 3.2 |
| 4 | H | 24 | ALA | 3.2 |
| 1 | C | 86 | LEU | 3.2 |
| 1 | A | 49 | GLY | 3.2 |
| 6 | R | 132 | VAL | 3.2 |
| 6 | U | 33 | LEU | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 5 | N | 125 | ALA | 3.2 |
| 5 | T | 24 | VAL | 3.2 |
| 5 | T | 120 | SER | 3.2 |
| 1 | A | 165 | ASN | 3.2 |
| 6 | R | 117 | ILE | 3.1 |
| 1 | A | 89 | GLU | 3.1 |
| 3 | J | 192 | TYR | 3.1 |
| 5 | Q | 102 | HIS | 3.1 |
| 6 | O | 140 | TYR | 3.1 |
| 5 | Q | 115 | SER | 3.1 |
| 5 | T | 97 | GLU | 3.1 |
| 4 | H | 45 | LEU | 3.1 |
| 6 | R | 152 | ASN | 3.1 |
| 1 | G | 178 | ILE | 3.1 |
| 6 | U | 120 | PRO | 3.1 |
| 3 | E | 181 | LEU | 3.1 |
| 1 | A | 261(D) | PRO | 3.0 |
| 6 | O | 151 | ASP | 3.0 |
| 1 | A | 50 | GLU | 3.0 |
| 1 | A | 244 | THR | 3.0 |
| 4 | K | 121 | VAL | 3.0 |
| 1 | G | 69 | THR | 3.0 |
| 2 | I | 171 | PHE | 3.0 |
| 6 | U | 37 | GLN | 3.0 |
| 1 | G | 185 | SER | 3.0 |
| 5 | N | 2 | VAL | 3.0 |
| 1 | G | 150 | GLU | 3.0 |
| 5 | T | 137 | ALA | 3.0 |
| 5 | Q | 133 | GLY | 3.0 |
| 5 | N | 100(E) | GLY | 3.0 |
| 1 | C | 83 | LYS | 3.0 |
| 6 | R | 209 | PHE | 3.0 |
| 5 | N | 35(A) | TRP | 3.0 |
| 5 | N | 119 | PRO | 3.0 |
| 1 | A | 12 | THR | 3.0 |
| 6 | U | 147 | GLN | 3.0 |
| 5 | T | 212 | GLU | 3.0 |
| 1 | C | 252 | ILE | 3.0 |
| 2 | D | 66 | ILE | 3.0 |
| 5 | T | 26 | GLY | 2.9 |
| 6 | R | 180 | THR | 2.9 |
| 1 | A | 153 | TRP | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 3 | J | 88 | CYS | 2.9 |
| 1 | G | 215 | PRO | 2.9 |
| 6 | U | 148 | TRP | 2.9 |
| 1 | G | 261(G) | ILE | 2.9 |
| 1 | C | 119 | ASP | 2.9 |
| 6 | U | 82 | ASP | 2.9 |
| 6 | R | 133 | VAL | 2.9 |
| 3 | E | 192 | TYR | 2.9 |
| 1 | A | 60 | ASP | 2.9 |
| 4 | F | 45 | LEU | 2.9 |
| 1 | G | 153 | TRP | 2.9 |
| 2 | I | 69 | GLU | 2.9 |
| 3 | J | 35 | TRP | 2.9 |
| 4 | H | 199 | GLY | 2.9 |
| 5 | T | 28 | SER | 2.9 |
| 6 | U | 119 | PRO | 2.9 |
| 4 | H | 127 | SER | 2.9 |
| 1 | G | 209 | TYR | 2.8 |
| 4 | F | 119 | PRO | 2.8 |
| 6 | U | 149 | LYS | 2.8 |
| 5 | N | 28 | SER | 2.8 |
| 1 | G | 232 | PHE | 2.8 |
| 5 | Q | 140 | CYS | 2.8 |
| 5 | Q | 71 | ILE | 2.8 |
| 5 | T | 46 | GLU | 2.8 |
| 1 | C | 122 | SER | 2.8 |
| 3 | E | 89 | GLN | 2.8 |
| 3 | E | 104 | LEU | 2.8 |
| 1 | G | 230 | ILE | 2.8 |
| 1 | G | 164 | LEU | 2.8 |
| 5 | T | 152 | VAL | 2.8 |
| 5 | T | 124 | LEU | 2.8 |
| 6 | U | 88 | CYS | 2.8 |
| 2 | D | 67 | GLU | 2.8 |
| 3 | L | 86 | TYR | 2.8 |
| 4 | H | 103 | TRP | 2.8 |
| 1 | A | 208 | LYS | 2.8 |
| 1 | A | 245 | PHE | 2.8 |
| 2 | B | 69 | GLU | 2.8 |
| 2 | D | 142 | HIS | 2.8 |
| 4 | H | 228 | LYS | 2.8 |
| 5 | T | 161 | SER | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | C | 158 | MET | 2.8 |
| 6 | R | 119 | PRO | 2.8 |
| 1 | C | 88 | ILE | 2.8 |
| 3 | L | 64 | GLY | 2.8 |
| 6 | O | 105 | GLU | 2.8 |
| 6 | U | 166 | GLN | 2.7 |
| 1 | C | 255 | ASP | 2.7 |
| 6 | O | 152 | ASN | 2.7 |
| 6 | R | 36 | PHE | 2.7 |
| 5 | N | 127 | SER | 2.7 |
| 5 | T | 25 | SER | 2.7 |
| 3 | J | 185 | ASP | 2.7 |
| 1 | C | 200 | LYS | 2.7 |
| 4 | K | 228 | LYS | 2.7 |
| 3 | J | 181 | LEU | 2.7 |
| 5 | T | 80 | LEU | 2.7 |
| 6 | U | 150 | VAL | 2.7 |
| 6 | U | 194 | CYS | 2.7 |
| 5 | Q | 2 | VAL | 2.7 |
| 6 | U | 64 | GLY | 2.7 |
| 4 | F | 102 | VAL | 2.7 |
| 6 | U | 91 | SER | 2.7 |
| 6 | R | 147 | GLN | 2.7 |
| 3 | E | 180 | THR | 2.7 |
| 5 | N | 136 | ALA | 2.6 |
| 5 | T | 100(H) | PRO | 2.6 |
| 5 | T | 138 | LEU | 2.6 |
| 5 | Q | 112 | SER | 2.6 |
| 2 | I | 173 | ILE | 2.6 |
| 1 | A | 133 | ASP | 2.6 |
| 6 | U | 51 | ALA | 2.6 |
| 1 | C | 165 | ASN | 2.6 |
| 4 | K | 24 | ALA | 2.6 |
| 1 | A | 100 | GLY | 2.6 |
| 1 | G | 297 | VAL | 2.6 |
| 1 | C | 306 | PRO | 2.6 |
| 5 | T | 187 | SER | 2.6 |
| 3 | E | 131 | SER | 2.6 |
| 6 | R | 129 | THR | 2.6 |
| 3 | E | 117 | ILE | 2.6 |
| 3 | J | 186 | TYR | 2.6 |
| 1 | G | 102 | PHE | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 6 | U | 181 | LEU | 2.6 |
| 5 | N | 52 | PHE | 2.6 |
| 6 | R | 90 | GLN | 2.6 |
| 1 | A | 325 | GLU | 2.6 |
| 6 | O | 144 | ALA | 2.6 |
| 1 | C | 167 | THR | 2.6 |
| 5 | Q | 135 | THR | 2.6 |
| 6 | R | 1 | ASP | 2.6 |
| 6 | R | 63 | SER | 2.6 |
| 6 | U | 117 | ILE | 2.6 |
| 1 | G | 195 | TYR | 2.6 |
| 5 | Q | 114 | ALA | 2.5 |
| 5 | Q | 18 | LEU | 2.5 |
| 5 | T | 79 | SER | 2.5 |
| 2 | D | 144 | CYS | 2.5 |
| 3 | E | 63 | SER | 2.5 |
| 5 | T | 121 | VAL | 2.5 |
| 6 | O | 73 | LEU | 2.5 |
| 6 | O | 149 | LYS | 2.5 |
| 6 | U | 13 | ALA | 2.5 |
| 1 | A | 67 | LEU | 2.5 |
| 4 | H | 221 | LYS | 2.5 |
| 4 | K | 37 | VAL | 2.5 |
| 4 | K | 34 | LEU | 2.5 |
| 5 | T | 180 | SER | 2.5 |
| 6 | R | 158 | ASN | 2.5 |
| 1 | G | 258 | THR | 2.5 |
| 5 | T | 125 | ALA | 2.5 |
| 6 | O | 23 | CYS | 2.5 |
| 6 | O | 71 | PHE | 2.5 |
| 5 | Q | 13 | LYS | 2.5 |
| 5 | Q | 19 | SER | 2.5 |
| 5 | N | 161 | SER | 2.5 |
| 1 | C | 280 | GLU | 2.5 |
| 4 | F | 221 | LYS | 2.5 |
| 4 | K | 38 | ARG | 2.5 |
| 6 | R | 64 | GLY | 2.5 |
| 1 | A | 248 | ASN | 2.5 |
| 1 | G | 261(C) | ALA | 2.5 |
| 4 | F | 67 | PHE | 2.5 |
| 4 | K | 94 | LYS | 2.5 |
| 1 | C | 242 | THR | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 2 | D | 171 | PHE | 2.5 |
| 5 | N | 100(D) | SER | 2.5 |
| 6 | U | 12 | SER | 2.5 |
| 6 | U | 185 | ASP | 2.5 |
| 1 | G | 13 | LEU | 2.5 |
| 1 | C | 180 | TRP | 2.4 |
| 5 | N | 141 | LEU | 2.4 |
| 1 | A | 261(G) | ILE | 2.4 |
| 5 | N | 94 | ARG | 2.4 |
| 2 | D | 70 | PHE | 2.4 |
| 2 | I | 73 | VAL | 2.4 |
| 5 | N | 1 | GLN | 2.4 |
| 5 | N | 47 | TRP | 2.4 |
| 5 | Q | 117 | LYS | 2.4 |
| 6 | U | 118 | PHE | 2.4 |
| 5 | Q | 113 | SER | 2.4 |
| 2 | I | 143 | LYS | 2.4 |
| 3 | L | 35 | TRP | 2.4 |
| 3 | J | 1 | GLU | 2.4 |
| 6 | U | 187 | GLU | 2.4 |
| 5 | T | 94 | ARG | 2.4 |
| 1 | C | 259 | PHE | 2.4 |
| 1 | A | 168 | TYR | 2.4 |
| 6 | O | 166 | GLN | 2.4 |
| 5 | T | 81 | ARG | 2.4 |
| 1 | G | 216 | SER | 2.4 |
| 3 | L | 36 | TYR | 2.4 |
| 1 | G | 158(B) | ASN | 2.4 |
| 4 | F | 34 | LEU | 2.4 |
| 2 | D | 65 | GLN | 2.4 |
| 3 | L | 34 | ALA | 2.4 |
| 4 | H | 206 | TYR | 2.4 |
| 6 | R | 33 | LEU | 2.4 |
| 6 | R | 118 | PHE | 2.4 |
| 1 | C | 248 | ASN | 2.4 |
| 4 | K | 208 | CYS | 2.4 |
| 6 | R | 194 | CYS | 2.4 |
| 5 | N | 34 | TYR | 2.4 |
| 5 | T | 143 | LYS | 2.4 |
| 5 | T | 30 | THR | 2.4 |
| 5 | N | 180 | SER | 2.3 |
| 6 | U | 183 | LYS | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5 | Q | 182 | VAL | 2.3 |
| 1 | G | 155 | SER | 2.3 |
| 1 | G | 160 | VAL | 2.3 |
| 5 | N | 24 | VAL | 2.3 |
| 5 | T | 103 | TRP | 2.3 |
| 4 | F | 78 | LEU | 2.3 |
| 3 | E | 1 | GLU | 2.3 |
| 6 | U | 205 | VAL | 2.3 |
| 1 | A | 237 | LEU | 2.3 |
| 2 | I | 27 | GLN | 2.3 |
| 5 | N | 80 | LEU | 2.3 |
| 6 | R | 52 | SER | 2.3 |
| 3 | E | 97 | THR | 2.3 |
| 6 | O | 66 | GLY | 2.3 |
| 3 | E | 47 | LEU | 2.3 |
| 5 | N | 32 | ASP | 2.3 |
| 6 | R | 51 | ALA | 2.3 |
| 3 | E | 146 | VAL | 2.3 |
| 5 | Q | 136 | ALA | 2.3 |
| 5 | T | 117 | LYS | 2.3 |
| 5 | Q | 12 | VAL | 2.3 |
| 5 | Q | 211 | VAL | 2.3 |
| 6 | R | 161 | GLU | 2.3 |
| 5 | T | 126 | PRO | 2.3 |
| 3 | E | 86 | TYR | 2.3 |
| 5 | N | 208 | ASP | 2.3 |
| 1 | A | 178 | ILE | 2.3 |
| 6 | R | 178 | THR | 2.3 |
| 3 | E | 32 | ASN | 2.3 |
| 6 | R | 34 | ASN | 2.3 |
| 6 | U | 80 | PRO | 2.3 |
| 2 | I | 142 | HIS | 2.3 |
| 3 | J | 46 | LEU | 2.3 |
| 4 | H | 121 | VAL | 2.3 |
| 6 | R | 22 | THR | 2.3 |
| 4 | F | 103 | TRP | 2.3 |
| 1 | A | 138 | ALA | 2.3 |
| 1 | G | 63 | SER | 2.3 |
| 4 | F | 205 | THR | 2.3 |
| 1 | A | 88 | ILE | 2.3 |
| 6 | U | 186 | TYR | 2.3 |
| 1 | A | 136 | THR | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 6 | O | 120 | PRO | 2.3 |
| 1 | A | 275 | ASP | 2.3 |
| 3 | L | 5 | THR | 2.3 |
| 1 | G | 257 | ALA | 2.2 |
| 4 | K | 139 | ALA | 2.2 |
| 1 | C | 179 | VAL | 2.2 |
| 1 | A | 206 | SER | 2.2 |
| 5 | Q | 80 | LEU | 2.2 |
| 3 | J | 89 | GLN | 2.2 |
| 4 | F | 225 | VAL | 2.2 |
| 5 | Q | 145 | TYR | 2.2 |
| 2 | I | 24 | PHE | 2.2 |
| 1 | G | 12 | THR | 2.2 |
| 1 | A | 130 | ILE | 2.2 |
| 1 | C | 70 | ILE | 2.2 |
| 5 | N | 121 | VAL | 2.2 |
| 1 | C | 231 | ASP | 2.2 |
| 1 | G | 247 | PHE | 2.2 |
| 2 | B | 68 | LYS | 2.2 |
| 2 | B | 171 | PHE | 2.2 |
| 3 | E | 209 | PHE | 2.2 |
| 3 | L | 181 | LEU | 2.2 |
| 1 | A | 232 | PHE | 2.2 |
| 3 | J | 37 | GLN | 2.2 |
| 4 | H | 140 | LEU | 2.2 |
| 1 | C | 132 | THR | 2.2 |
| 4 | F | 38 | ARG | 2.2 |
| 1 | A | 269 | GLN | 2.2 |
| 1 | A | 236 | LEU | 2.2 |
| 6 | O | 132 | VAL | 2.2 |
| 4 | K | 166 | LEU | 2.2 |
| 1 | A | 247 | PHE | 2.2 |
| 6 | O | 46 | LEU | 2.2 |
| 5 | Q | 196 | CYS | 2.2 |
| 5 | N | 27 | VAL | 2.2 |
| 1 | A | 11 | ALA | 2.2 |
| 2 | D | 128 | GLU | 2.2 |
| 6 | U | 41 | GLY | 2.2 |
| 6 | R | 4 | MET | 2.2 |
| 6 | R | 148 | TRP | 2.2 |
| 6 | U | 213 | GLU | 2.2 |
| 1 | C | 183 | HIS | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 1 | G | 260 | LEU | 2.2 |
| 6 | U | 206 | THR | 2.2 |
| 1 | C | 47 | SER | 2.2 |
| 1 | G | 157 | SER | 2.2 |
| 5 | Q | 194 | TYR | 2.2 |
| 1 | A | 123 | MET | 2.1 |
| 1 | G | 37 | THR | 2.1 |
| 1 | A | 215 | PRO | 2.1 |
| 6 | O | 146 | VAL | 2.1 |
| 5 | N | 58 | ASN | 2.1 |
| 6 | U | 79 | GLN | 2.1 |
| 1 | G | 38 | ASN | 2.1 |
| 6 | O | 141 | PRO | 2.1 |
| 4 | H | 100(H) | TYR | 2.1 |
| 6 | R | 208 | SER | 2.1 |
| 1 | A | 224 | ASN | 2.1 |
| 4 | F | 93 | ALA | 2.1 |
| 1 | A | 83 | LYS | 2.1 |
| 1 | G | 173 | LYS | 2.1 |
| 5 | N | 100(A) | TYR | 2.1 |
| 5 | T | 98 | ASP | 2.1 |
| 5 | N | 56 | ASP | 2.1 |
| 6 | R | 23 | CYS | 2.1 |
| 6 | R | 112 | ALA | 2.1 |
| 6 | U | 184 | ALA | 2.1 |
| 5 | T | 114 | ALA | 2.1 |
| 4 | H | 101 | ASP | 2.1 |
| 3 | E | 4 | MET | 2.1 |
| 6 | U | 1 | ASP | 2.1 |
| 5 | N | 181 | VAL | 2.1 |
| 6 | R | 104 | VAL | 2.1 |
| 3 | E | 62 | PHE | 2.1 |
| 1 | C | 102 | PHE | 2.1 |
| 6 | R | 48 | ILE | 2.1 |
| 4 | K | 165 | ALA | 2.1 |
| 5 | Q | 207 | VAL | 2.1 |
| 1 | C | 262 | ASN | 2.1 |
| 3 | L | 29 | VAL | 2.1 |
| 4 | F | 121 | VAL | 2.1 |
| 5 | Q | 198 | VAL | 2.1 |
| 5 | N | 57 | THR | 2.1 |
| 1 | C | 273 | GLN | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|--------|------|------|
| 5 | Q | 103 | TRP | 2.0 |
| 6 | R | 89 | GLN | 2.0 |
| 3 | E | 45 | ARG | 2.0 |
| 6 | O | 108 | ARG | 2.0 |
| 5 | Q | 1 | GLN | 2.0 |
| 6 | R | 83 | PHE | 2.0 |
| 1 | G | 245 | PHE | 2.0 |
| 4 | F | 92 | CYS | 2.0 |
| 5 | N | 38 | ARG | 2.0 |
| 5 | T | 7 | SER | 2.0 |
| 4 | H | 166 | LEU | 2.0 |
| 2 | B | 7 | ALA | 2.0 |
| 4 | K | 199 | GLY | 2.0 |
| 5 | T | 9 | PRO | 2.0 |
| 5 | T | 182 | VAL | 2.0 |
| 1 | G | 148 | TYR | 2.0 |
| 3 | L | 87 | TYR | 2.0 |
| 5 | Q | 100(E) | GLY | 2.0 |
| 4 | K | 109 | VAL | 2.0 |
| 2 | B | 128 | GLU | 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.