



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 11:39 AM EDT

PDB ID : 3T4A
Title : Structure of a truncated form of Staphylococcal Complement Inhibitor B bound to human C3c at 3.4 Angstrom resolution
Authors : Garcia, B.L.; Geisbrecht, B.V.; Summers, B.J.
Deposited on : 2011-07-25
Resolution : 3.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.35
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) : 2.35

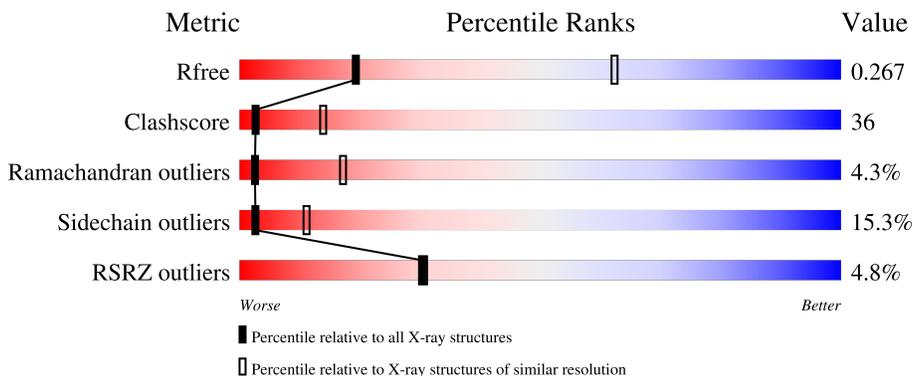
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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.



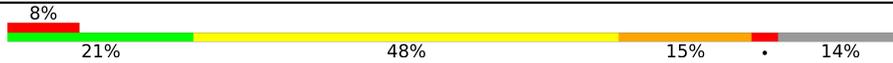
| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1026 (3.48-3.32) |
| Clashscore | 141614 | 1055 (3.48-3.32) |
| Ramachandran outliers | 138981 | 1038 (3.48-3.32) |
| Sidechain outliers | 138945 | 1038 (3.48-3.32) |
| RSRZ outliers | 127900 | 2173 (3.50-3.30) |

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 | 645 | <div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 53%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 53% 36% 10% .</p> |
| 1 | D | 645 | <div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 53%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 53% 36% 9% .</p> |
| 2 | B | 206 | <div style="display: flex; align-items: center;"> <div style="width: 49%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">49% 33% 7% 11%</p> |
| 2 | E | 206 | <div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 52%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">% 52% 30% 6% 11%</p> |
| 3 | C | 343 | <div style="display: flex; align-items: center;"> <div style="width: 19%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">19% 21% 50% 13% . 14%</p> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 3 | F | 343 |  |
| 4 | G | 73 |  |
| 4 | H | 73 |  |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18730 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 Complement C3 beta chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 1 | A | 633 | 4931 | 3141 | 833 | 942 | 15 | 0 | 0 | 0 |
| 1 | D | 633 | 4931 | 3141 | 833 | 942 | 15 | 0 | 0 | 0 |

- Molecule 2 is a protein called Complement C3c alpha' chain fragment 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 2 | B | 183 | 1480 | 950 | 249 | 276 | 5 | 0 | 0 | 0 |
| 2 | E | 183 | 1480 | 950 | 249 | 276 | 5 | 0 | 0 | 0 |

- Molecule 3 is a protein called Complement C3c alpha' chain fragment 2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 3 | C | 296 | 2407 | 1517 | 395 | 475 | 20 | 0 | 0 | 0 |
| 3 | F | 296 | 2407 | 1517 | 395 | 475 | 20 | 0 | 0 | 0 |

- Molecule 4 is a protein called Fibrinogen-binding protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 4 | G | 68 | 547 | 348 | 94 | 102 | 3 | 0 | 0 | 0 |
| 4 | H | 68 | 547 | 348 | 94 | 102 | 3 | 0 | 0 | 0 |

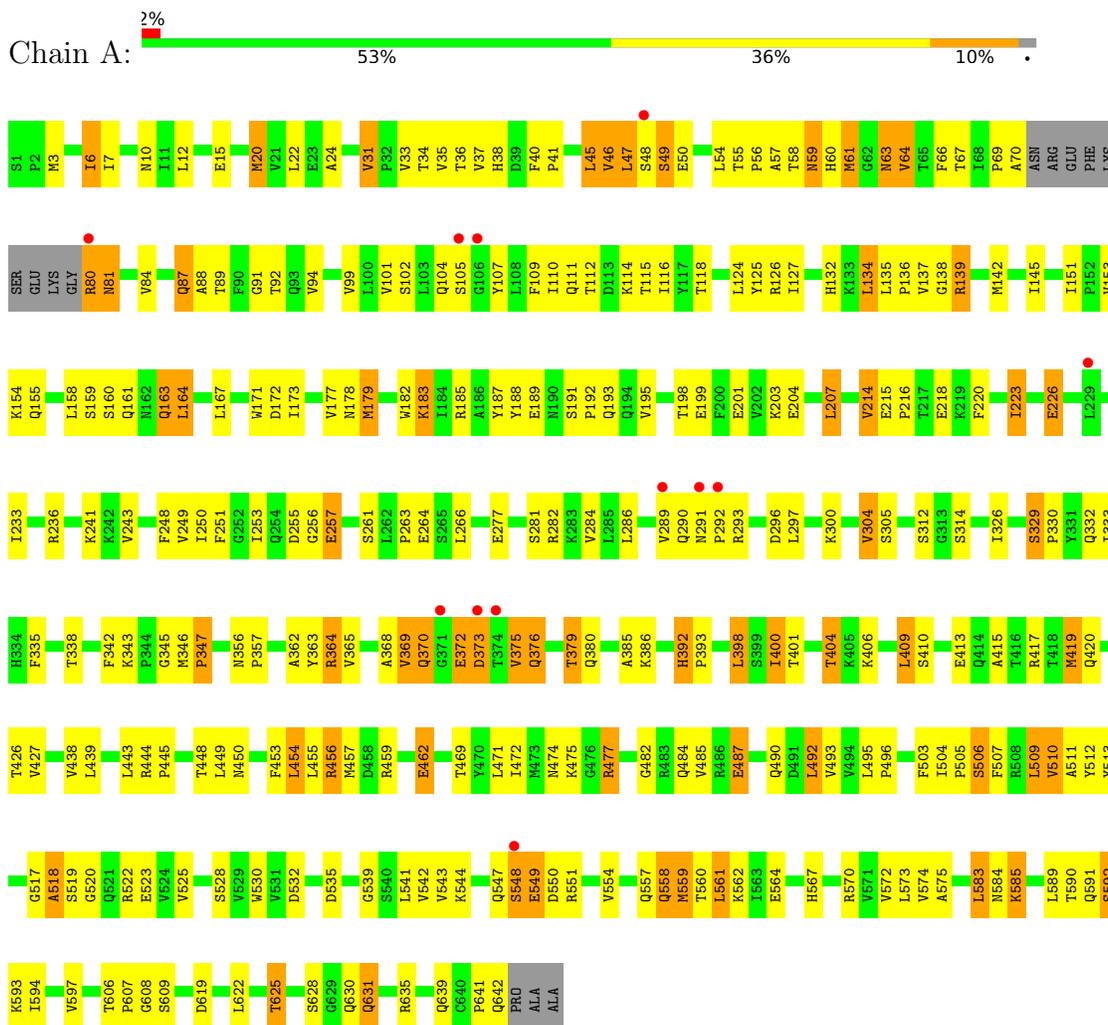
There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| G | 13 | GLY | - | expression tag | UNP Q99UU9 |
| G | 14 | SER | - | expression tag | UNP Q99UU9 |
| G | 15 | THR | - | expression tag | UNP Q99UU9 |
| G | 16 | GLY | - | expression tag | UNP Q99UU9 |
| G | 17 | SER | - | expression tag | UNP Q99UU9 |
| H | 13 | GLY | - | expression tag | UNP Q99UU9 |
| H | 14 | SER | - | expression tag | UNP Q99UU9 |
| H | 15 | THR | - | expression tag | UNP Q99UU9 |
| H | 16 | GLY | - | expression tag | UNP Q99UU9 |
| H | 17 | SER | - | expression tag | UNP Q99UU9 |

3 Residue-property plots

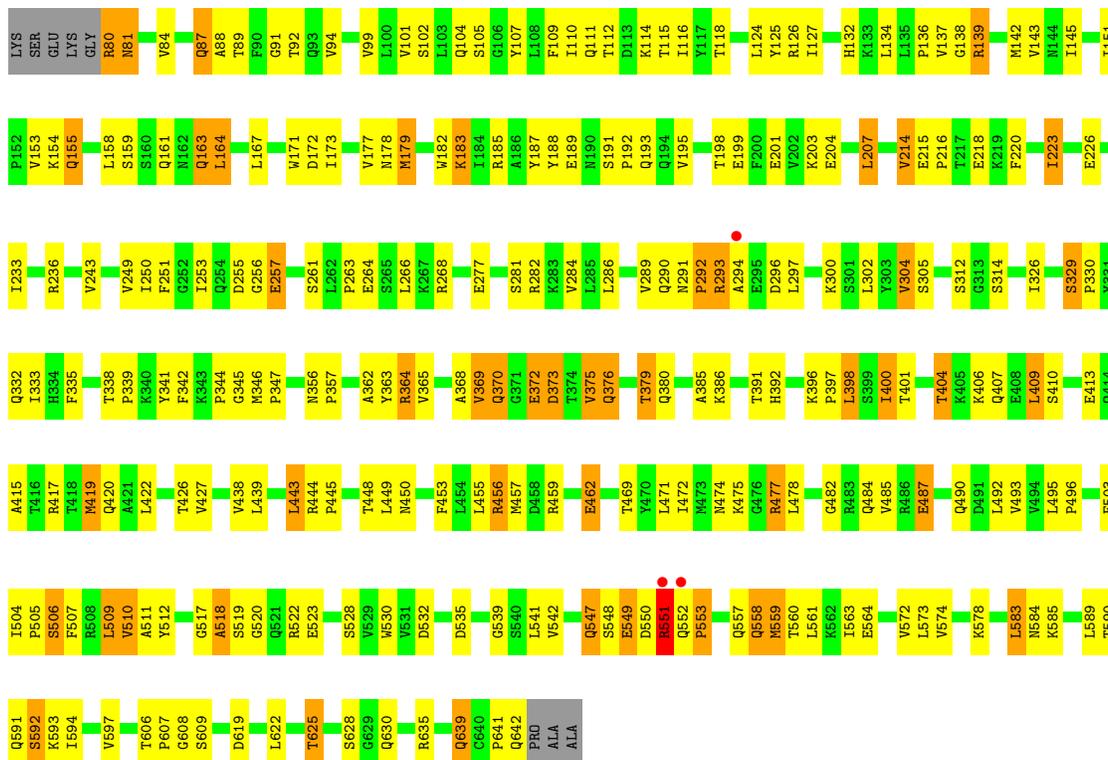
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Complement C3 beta chain



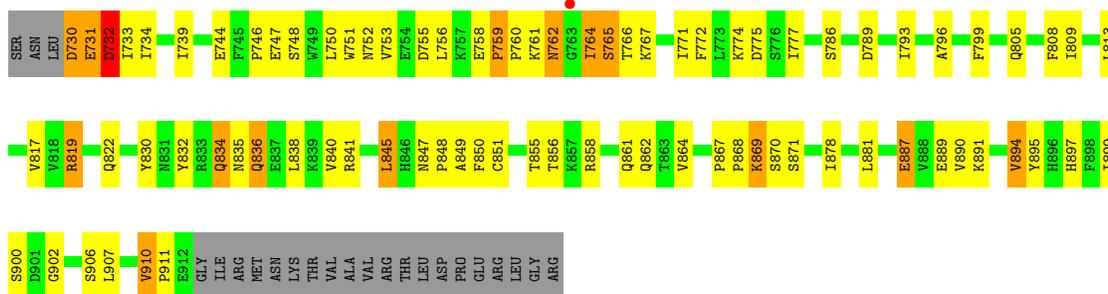
- Molecule 1: Complement C3 beta chain





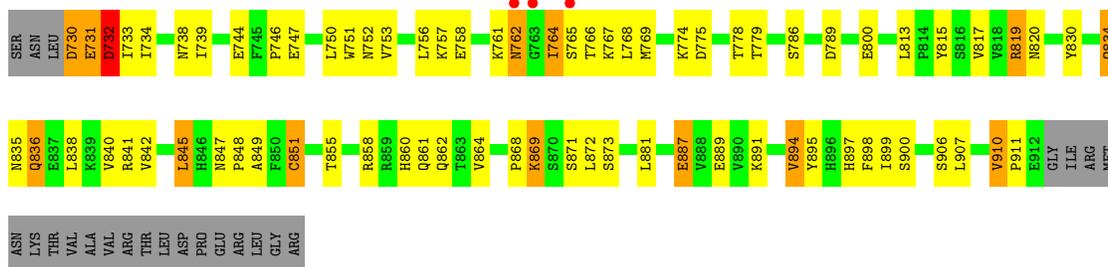
• Molecule 2: Complement C3c alpha' chain fragment 1

Chain B: 49% 33% 7% 11%

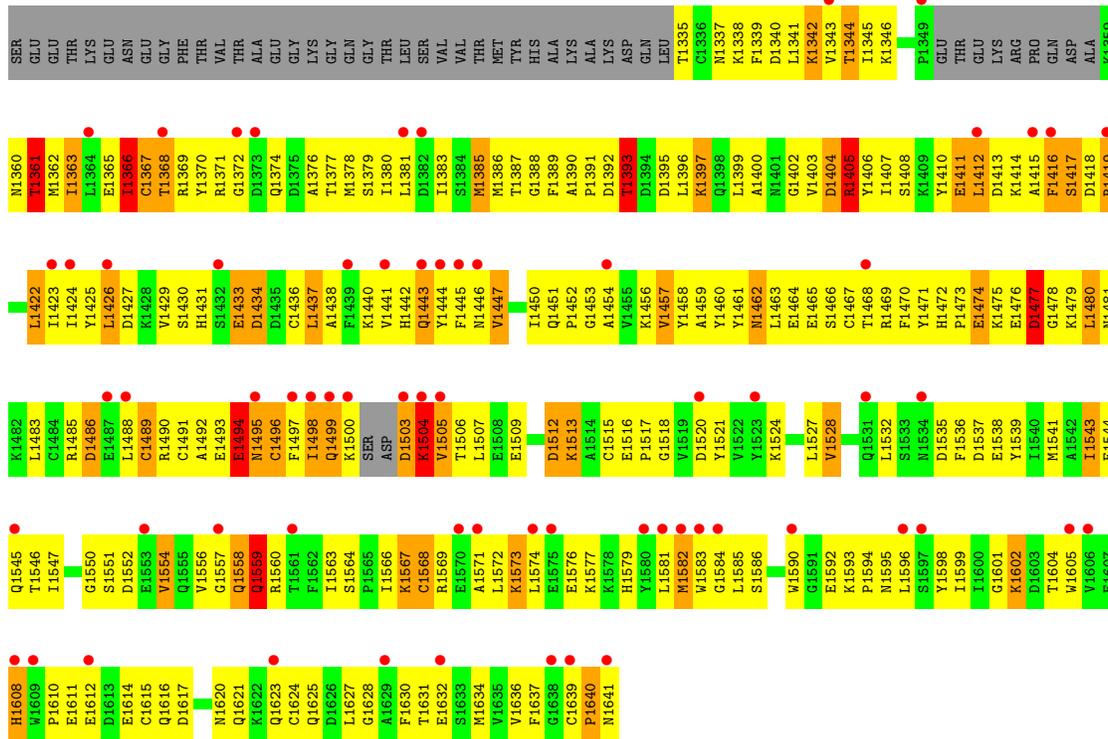


• Molecule 2: Complement C3c alpha' chain fragment 1

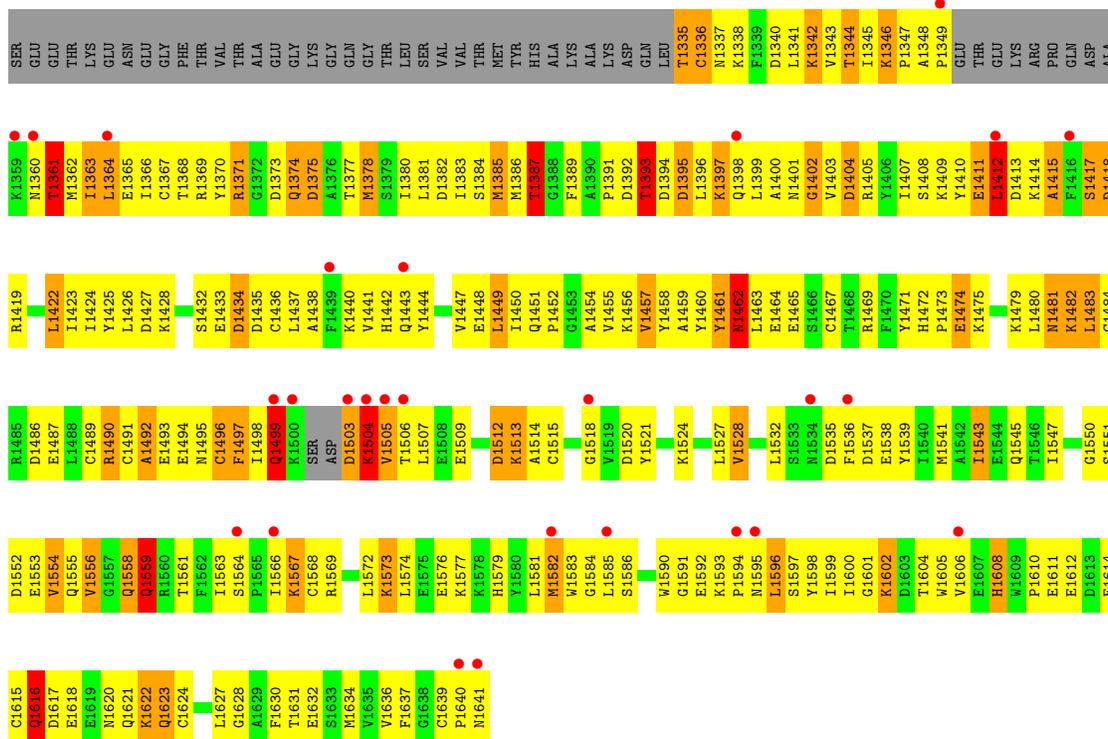
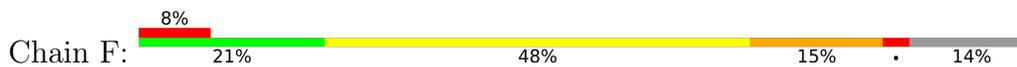
Chain E: % 52% 30% 6% 11%



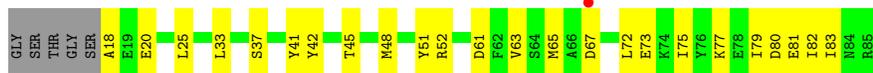
• Molecule 3: Complement C3c alpha' chain fragment 2



• Molecule 3: Complement C3c alpha' chain fragment 2



- Molecule 4: Fibrinogen-binding protein



- Molecule 4: Fibrinogen-binding protein



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 103.30Å 165.44Å 203.12Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 32.71 – 3.40 50.06 – 3.40 | Depositor EDS |
| % Data completeness (in resolution range) | 92.6 (32.71-3.40) 91.6 (50.06-3.40) | Depositor EDS |
| R_{merge} | 0.16 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 4.25 (at 3.40Å) | Xtrriage |
| Refinement program | PHENIX 1.7_650 | Depositor |
| R, R_{free} | 0.229 , 0.270 0.224 , 0.267 | Depositor DCC |
| R_{free} test set | 2000 reflections (4.27%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 59.0 | Xtrriage |
| Anisotropy | 0.158 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 39.9 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtrriage |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| F_o, F_c correlation | 0.89 | EDS |
| Total number of atoms | 18730 | wwPDB-VP |
| Average B, all atoms (Å ²) | 67.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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 [i](#)

5.1 Standard geometry [i](#)

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 | 0.52 | 1/5030 (0.0%) | 0.69 | 0/6837 |
| 1 | D | 0.51 | 0/5030 | 0.68 | 0/6837 |
| 2 | B | 0.50 | 0/1512 | 0.65 | 0/2055 |
| 2 | E | 0.52 | 0/1512 | 0.67 | 0/2055 |
| 3 | C | 0.53 | 1/2453 (0.0%) | 0.72 | 4/3305 (0.1%) |
| 3 | F | 0.65 | 1/2453 (0.0%) | 0.78 | 0/3305 |
| 4 | G | 0.53 | 0/553 | 0.65 | 0/741 |
| 4 | H | 0.52 | 0/553 | 0.64 | 0/741 |
| All | All | 0.54 | 3/19096 (0.0%) | 0.70 | 4/25876 (0.0%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3 | F | 1623 | GLN | C-N | -5.78 | 1.20 | 1.34 |
| 3 | C | 1391 | PRO | C-N | -5.63 | 1.21 | 1.34 |
| 1 | A | 631 | GLN | C-N | -5.54 | 1.21 | 1.34 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3 | C | 1419 | ARG | CB-CA-C | -5.99 | 98.41 | 110.40 |
| 3 | C | 1447 | VAL | N-CA-CB | 5.88 | 124.42 | 111.50 |
| 3 | C | 1405 | ARG | N-CA-CB | 5.21 | 119.99 | 110.60 |
| 3 | C | 1498 | ILE | CB-CA-C | 5.06 | 121.72 | 111.60 |

There are no chirality outliers.

There are no planarity outliers.

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 | 4931 | 0 | 4993 | 292 | 0 |
| 1 | D | 4931 | 0 | 4993 | 275 | 0 |
| 2 | B | 1480 | 0 | 1501 | 98 | 0 |
| 2 | E | 1480 | 0 | 1501 | 89 | 0 |
| 3 | C | 2407 | 0 | 2316 | 350 | 0 |
| 3 | F | 2407 | 0 | 2315 | 287 | 0 |
| 4 | G | 547 | 0 | 568 | 19 | 0 |
| 4 | H | 547 | 0 | 568 | 30 | 0 |
| All | All | 18730 | 0 | 18755 | 1362 | 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 36.

All (1362) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:1389:PHE:CD2 | 3:C:1443:GLN:HB2 | 1.46 | 1.50 |
| 3:C:1381:LEU:HD13 | 3:C:1383:ILE:CG1 | 1.38 | 1.47 |
| 3:C:1381:LEU:CD1 | 3:C:1383:ILE:HG13 | 1.47 | 1.41 |
| 1:A:346:MET:HE3 | 1:A:456:ARG:CB | 1.54 | 1.36 |
| 3:C:1379:SER:C | 3:C:1380:ILE:HD12 | 1.44 | 1.36 |
| 1:A:253:ILE:HD12 | 1:A:289:VAL:CG1 | 1.57 | 1.32 |
| 3:F:1494:GLU:CG | 3:F:1602:LYS:HD3 | 1.60 | 1.31 |
| 2:E:758:GLU:OE2 | 2:E:767:LYS:HB2 | 1.29 | 1.28 |
| 3:C:1366:ILE:O | 3:C:1367:CYS:SG | 1.94 | 1.26 |
| 3:C:1376:ALA:HB3 | 3:C:1429:VAL:CG2 | 1.69 | 1.23 |
| 3:C:1396:LEU:HB3 | 3:C:1412:LEU:CD1 | 1.67 | 1.22 |
| 3:C:1389:PHE:CE2 | 3:C:1443:GLN:HB2 | 1.77 | 1.18 |
| 1:A:346:MET:CE | 1:A:456:ARG:CB | 2.23 | 1.17 |
| 3:C:1389:PHE:CE2 | 3:C:1443:GLN:CB | 2.27 | 1.17 |
| 3:C:1381:LEU:HD13 | 3:C:1383:ILE:CD1 | 1.76 | 1.16 |
| 3:C:1389:PHE:CZ | 3:C:1443:GLN:HB3 | 1.79 | 1.16 |
| 3:C:1365:GLU:O | 3:C:1366:ILE:HG12 | 1.47 | 1.14 |
| 1:D:253:ILE:CD1 | 1:D:302:LEU:CD2 | 2.24 | 1.14 |
| 3:C:1396:LEU:HB3 | 3:C:1412:LEU:HD11 | 1.30 | 1.13 |
| 3:C:1552:ASP:OD1 | 3:C:1554:VAL:HG12 | 1.47 | 1.13 |
| 3:C:1390:ALA:HB3 | 3:C:1416:PHE:CD1 | 1.84 | 1.12 |
| 3:C:1404:ASP:HA | 3:C:1427:ASP:OD1 | 1.49 | 1.11 |
| 1:A:346:MET:CE | 1:A:456:ARG:HB3 | 1.80 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:392:HIS:HB3 | 1:A:393:PRO:CD | 1.80 | 1.10 |
| 1:A:253:ILE:HD12 | 1:A:289:VAL:HG11 | 1.32 | 1.10 |
| 1:D:253:ILE:HD13 | 1:D:302:LEU:CD2 | 1.82 | 1.09 |
| 1:A:253:ILE:CD1 | 1:A:289:VAL:CG1 | 2.31 | 1.09 |
| 1:A:253:ILE:CD1 | 1:A:289:VAL:HG11 | 1.81 | 1.09 |
| 3:C:1389:PHE:CD2 | 3:C:1443:GLN:CB | 2.36 | 1.07 |
| 1:A:392:HIS:HB3 | 1:A:393:PRO:HD2 | 1.10 | 1.06 |
| 3:C:1376:ALA:HB3 | 3:C:1429:VAL:HG22 | 1.29 | 1.05 |
| 3:C:1404:ASP:HA | 3:C:1427:ASP:CG | 1.76 | 1.05 |
| 3:F:1494:GLU:HG2 | 3:F:1602:LYS:HD3 | 1.07 | 1.04 |
| 3:F:1618:GLU:CA | 3:F:1621:GLN:HG3 | 1.88 | 1.03 |
| 3:F:1494:GLU:HG2 | 3:F:1602:LYS:CD | 1.88 | 1.03 |
| 1:D:547:GLN:O | 1:D:547:GLN:HG2 | 1.54 | 1.03 |
| 1:A:346:MET:CE | 1:A:456:ARG:HB2 | 1.86 | 1.02 |
| 3:F:1483:LEU:HD21 | 3:F:1590:TRP:CE2 | 1.94 | 1.02 |
| 3:F:1618:GLU:HA | 3:F:1621:GLN:HG3 | 1.10 | 1.02 |
| 1:A:289:VAL:O | 3:F:1594:PRO:HG2 | 1.59 | 1.02 |
| 1:A:454:LEU:HD22 | 1:A:492:LEU:HD12 | 1.37 | 1.02 |
| 1:D:55:THR:HG22 | 1:D:57:ALA:H | 1.25 | 1.01 |
| 1:A:253:ILE:HD12 | 1:A:289:VAL:HG13 | 1.43 | 1.01 |
| 3:F:1504:LYS:O | 3:F:1505:VAL:HG22 | 1.61 | 1.01 |
| 1:A:55:THR:HG22 | 1:A:57:ALA:H | 1.25 | 1.00 |
| 3:C:1475:LYS:HE2 | 3:C:1493:GLU:OE2 | 1.61 | 1.00 |
| 3:F:1618:GLU:HA | 3:F:1621:GLN:CG | 1.90 | 1.00 |
| 3:C:1504:LYS:O | 3:C:1505:VAL:HG22 | 1.61 | 0.99 |
| 1:D:253:ILE:CD1 | 1:D:302:LEU:HD21 | 1.93 | 0.99 |
| 3:C:1343:VAL:HG22 | 3:C:1366:ILE:HG23 | 1.44 | 0.98 |
| 1:A:549:GLU:HG2 | 1:A:550:ASP:H | 1.28 | 0.98 |
| 3:C:1361:THR:HB | 3:C:1442:HIS:ND1 | 1.78 | 0.98 |
| 1:D:3:MET:HE3 | 1:D:522:ARG:HG2 | 1.46 | 0.97 |
| 3:C:1367:CYS:HB3 | 3:C:1434:ASP:OD2 | 1.65 | 0.97 |
| 3:F:1543:ILE:HD12 | 3:F:1554:VAL:HG21 | 1.43 | 0.96 |
| 1:A:3:MET:HE3 | 1:A:522:ARG:HG2 | 1.45 | 0.96 |
| 3:C:1381:LEU:CD1 | 3:C:1383:ILE:CD1 | 2.42 | 0.96 |
| 3:F:1341:LEU:HD21 | 3:F:1455:VAL:HG12 | 1.45 | 0.96 |
| 3:C:1378:MET:HA | 3:C:1427:ASP:O | 1.64 | 0.96 |
| 3:C:1488:LEU:HD23 | 3:C:1590:TRP:CH2 | 2.02 | 0.95 |
| 1:D:63:ASN:O | 1:D:64:VAL:HG13 | 1.68 | 0.93 |
| 1:A:63:ASN:O | 1:A:64:VAL:HG13 | 1.68 | 0.93 |
| 3:F:1483:LEU:HD12 | 3:F:1484:CYS:N | 1.84 | 0.93 |
| 3:C:1340:ASP:O | 3:C:1368:THR:HA | 1.68 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:1381:LEU:CD1 | 3:C:1383:ILE:CG1 | 2.21 | 0.92 |
| 3:C:1379:SER:O | 3:C:1380:ILE:HD12 | 1.66 | 0.92 |
| 3:C:1389:PHE:CG | 3:C:1443:GLN:HB2 | 2.04 | 0.92 |
| 3:C:1365:GLU:HG2 | 3:C:1366:ILE:N | 1.84 | 0.92 |
| 3:C:1380:ILE:CG2 | 3:C:1423:ILE:CG2 | 2.48 | 0.92 |
| 1:A:454:LEU:CD2 | 1:A:492:LEU:HD12 | 2.01 | 0.91 |
| 1:A:290:GLN:O | 1:A:290:GLN:HG3 | 1.70 | 0.91 |
| 1:D:372:GLU:HA | 1:D:373:ASP:CB | 1.99 | 0.91 |
| 1:A:292:PRO:HB3 | 3:F:1553:GLU:HB3 | 1.50 | 0.91 |
| 1:A:372:GLU:HA | 1:A:373:ASP:CB | 1.99 | 0.91 |
| 3:C:1386:MET:HA | 3:C:1451:GLN:O | 1.70 | 0.90 |
| 3:F:1381:LEU:HD23 | 3:F:1457:VAL:CG1 | 2.01 | 0.90 |
| 3:C:1379:SER:C | 3:C:1380:ILE:CD1 | 2.39 | 0.90 |
| 3:F:1407:ILE:HD11 | 3:F:1424:ILE:HG12 | 1.53 | 0.90 |
| 3:C:1376:ALA:HB3 | 3:C:1429:VAL:HG21 | 1.50 | 0.90 |
| 3:F:1593:LYS:N | 3:F:1596:LEU:CD2 | 2.35 | 0.89 |
| 3:C:1381:LEU:HD12 | 3:C:1383:ILE:HG13 | 1.54 | 0.89 |
| 2:E:764:ILE:HG22 | 2:E:764:ILE:O | 1.72 | 0.89 |
| 1:D:541:LEU:HD13 | 2:E:786:SER:HB3 | 1.53 | 0.89 |
| 3:C:1381:LEU:HD13 | 3:C:1383:ILE:HG13 | 0.93 | 0.89 |
| 1:A:136:PRO:HD2 | 2:B:789:ASP:HA | 1.54 | 0.89 |
| 1:A:372:GLU:CA | 1:A:373:ASP:HB2 | 2.03 | 0.88 |
| 1:D:372:GLU:CA | 1:D:373:ASP:HB2 | 2.03 | 0.88 |
| 3:F:1494:GLU:HG3 | 3:F:1602:LYS:HD3 | 1.54 | 0.88 |
| 1:D:372:GLU:N | 1:D:373:ASP:HB2 | 1.88 | 0.88 |
| 1:A:372:GLU:N | 1:A:373:ASP:HB2 | 1.88 | 0.88 |
| 2:E:819:ARG:HG2 | 2:E:819:ARG:HH11 | 1.39 | 0.88 |
| 1:A:24:ALA:HB3 | 1:A:60:HIS:HB3 | 1.56 | 0.88 |
| 1:D:24:ALA:HB3 | 1:D:60:HIS:HB3 | 1.56 | 0.87 |
| 3:C:1376:ALA:CB | 3:C:1429:VAL:CG2 | 2.53 | 0.87 |
| 2:E:758:GLU:OE2 | 2:E:767:LYS:CB | 2.20 | 0.86 |
| 1:A:105:SER:HB3 | 1:A:139:ARG:HE | 1.40 | 0.86 |
| 3:C:1404:ASP:HB3 | 3:C:1427:ASP:HB2 | 1.55 | 0.86 |
| 2:E:734:ILE:HA | 4:H:51:TYR:HE1 | 1.40 | 0.86 |
| 3:C:1396:LEU:CB | 3:C:1412:LEU:HD11 | 2.06 | 0.86 |
| 1:A:392:HIS:CB | 1:A:393:PRO:HD2 | 2.00 | 0.86 |
| 3:F:1462:ASN:ND2 | 3:F:1464:GLU:H | 1.74 | 0.85 |
| 3:F:1593:LYS:N | 3:F:1596:LEU:HD23 | 1.91 | 0.85 |
| 3:C:1475:LYS:CE | 3:C:1493:GLU:OE2 | 2.24 | 0.85 |
| 3:C:1365:GLU:HG2 | 3:C:1366:ILE:H | 1.40 | 0.85 |
| 1:A:241:LYS:HG3 | 2:B:832:TYR:CE2 | 2.11 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:819:ARG:HH11 | 2:B:819:ARG:HG2 | 1.41 | 0.84 |
| 3:C:1367:CYS:CB | 3:C:1434:ASP:OD2 | 2.25 | 0.84 |
| 3:F:1592:GLU:CA | 3:F:1596:LEU:HD23 | 2.06 | 0.84 |
| 3:C:1380:ILE:HG21 | 3:C:1423:ILE:CG2 | 2.07 | 0.84 |
| 1:D:290:GLN:O | 1:D:290:GLN:HG2 | 1.77 | 0.84 |
| 3:F:1592:GLU:C | 3:F:1596:LEU:HD23 | 1.98 | 0.84 |
| 3:C:1381:LEU:HD12 | 3:C:1381:LEU:O | 1.77 | 0.84 |
| 1:A:549:GLU:HG2 | 1:A:550:ASP:N | 1.93 | 0.83 |
| 1:A:346:MET:HE3 | 1:A:456:ARG:HB3 | 0.87 | 0.83 |
| 1:D:69:PRO:HA | 1:D:70:ALA:HB3 | 1.61 | 0.83 |
| 3:C:1389:PHE:CE1 | 3:C:1443:GLN:HB3 | 2.13 | 0.82 |
| 3:C:1552:ASP:OD1 | 3:C:1554:VAL:CG1 | 2.25 | 0.82 |
| 1:D:105:SER:HB3 | 1:D:139:ARG:HE | 1.41 | 0.82 |
| 1:A:281:SER:OG | 1:A:284:VAL:HG23 | 1.79 | 0.82 |
| 3:C:1389:PHE:HA | 3:C:1443:GLN:HA | 1.59 | 0.82 |
| 3:F:1462:ASN:C | 3:F:1462:ASN:HD22 | 1.84 | 0.82 |
| 1:D:253:ILE:HD13 | 1:D:302:LEU:HD22 | 1.62 | 0.82 |
| 1:D:281:SER:OG | 1:D:284:VAL:HG23 | 1.80 | 0.81 |
| 1:D:10:ASN:HB3 | 1:D:635:ARG:HD3 | 1.62 | 0.81 |
| 1:A:69:PRO:HA | 1:A:70:ALA:HB3 | 1.61 | 0.81 |
| 3:C:1552:ASP:CG | 3:C:1554:VAL:HG12 | 2.00 | 0.81 |
| 3:C:1367:CYS:HB3 | 3:C:1434:ASP:CG | 2.01 | 0.81 |
| 1:A:10:ASN:HB3 | 1:A:635:ARG:HD3 | 1.62 | 0.81 |
| 3:C:1433:GLU:O | 3:C:1434:ASP:HB2 | 1.81 | 0.80 |
| 1:A:329:SER:HB2 | 1:A:413:GLU:O | 1.81 | 0.80 |
| 1:A:6:ILE:HD13 | 1:A:22:LEU:HD23 | 1.64 | 0.80 |
| 1:A:628:SER:HB2 | 1:A:630:GLN:OE1 | 1.80 | 0.80 |
| 3:C:1443:GLN:HG2 | 3:C:1443:GLN:O | 1.82 | 0.80 |
| 1:D:329:SER:HB2 | 1:D:413:GLU:O | 1.81 | 0.80 |
| 3:C:1343:VAL:HG22 | 3:C:1366:ILE:CG2 | 2.12 | 0.79 |
| 1:D:628:SER:HB2 | 1:D:630:GLN:OE1 | 1.80 | 0.79 |
| 1:A:104:GLN:O | 1:A:132:HIS:HE1 | 1.66 | 0.79 |
| 3:C:1396:LEU:CB | 3:C:1412:LEU:CD1 | 2.57 | 0.79 |
| 1:D:6:ILE:HD13 | 1:D:22:LEU:HD23 | 1.64 | 0.79 |
| 2:B:836:GLN:NE2 | 2:B:897:HIS:HE1 | 1.79 | 0.79 |
| 3:C:1495:ASN:HD22 | 3:C:1496:CYS:N | 1.80 | 0.79 |
| 3:C:1454:ALA:HB2 | 3:C:1470:PHE:CE2 | 2.16 | 0.79 |
| 1:D:547:GLN:O | 1:D:547:GLN:CG | 2.30 | 0.79 |
| 1:A:207:LEU:HD21 | 2:B:747:GLU:HG2 | 1.64 | 0.78 |
| 3:C:1381:LEU:HD13 | 3:C:1383:ILE:HD11 | 1.64 | 0.78 |
| 3:F:1450:ILE:HD11 | 3:F:1472:HIS:CE1 | 2.17 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:1380:ILE:HG23 | 3:C:1423:ILE:HG22 | 1.63 | 0.78 |
| 3:C:1424:ILE:HG22 | 3:C:1426:LEU:CD1 | 2.14 | 0.78 |
| 1:D:104:GLN:O | 1:D:132:HIS:HE1 | 1.66 | 0.78 |
| 1:D:552:GLN:HB3 | 1:D:553:PRO:HD2 | 1.63 | 0.78 |
| 3:C:1390:ALA:CB | 3:C:1416:PHE:CD1 | 2.66 | 0.78 |
| 3:F:1590:TRP:O | 3:F:1596:LEU:HA | 1.83 | 0.78 |
| 4:G:61:ASP:O | 4:G:65:MET:HG3 | 1.82 | 0.78 |
| 3:C:1365:GLU:O | 3:C:1366:ILE:CG1 | 2.30 | 0.78 |
| 3:F:1381:LEU:HD23 | 3:F:1457:VAL:HG13 | 1.66 | 0.78 |
| 1:A:45:LEU:HD21 | 1:A:48:SER:HB3 | 1.66 | 0.77 |
| 1:D:293:ARG:O | 1:D:296:ASP:HB2 | 1.84 | 0.77 |
| 2:B:734:ILE:HA | 4:G:51:TYR:HE1 | 1.48 | 0.77 |
| 1:D:549:GLU:O | 1:D:550:ASP:HB2 | 1.85 | 0.77 |
| 3:C:1480:LEU:HB3 | 3:C:1493:GLU:HG3 | 1.67 | 0.77 |
| 3:F:1397:LYS:H | 3:F:1397:LYS:HD3 | 1.49 | 0.77 |
| 1:A:136:PRO:CD | 2:B:789:ASP:HA | 2.14 | 0.77 |
| 1:D:45:LEU:HD21 | 1:D:48:SER:HB3 | 1.66 | 0.77 |
| 3:F:1344:THR:CG2 | 3:F:1346:LYS:HE2 | 2.15 | 0.77 |
| 3:C:1495:ASN:O | 3:C:1496:CYS:CB | 2.32 | 0.76 |
| 4:H:61:ASP:O | 4:H:65:MET:HG3 | 1.86 | 0.76 |
| 3:C:1338:LYS:HD3 | 3:C:1465:GLU:HB2 | 1.67 | 0.76 |
| 3:C:1543:ILE:HD12 | 3:C:1554:VAL:HG21 | 1.67 | 0.76 |
| 3:C:1380:ILE:CG2 | 3:C:1423:ILE:HG22 | 2.14 | 0.76 |
| 1:A:289:VAL:O | 3:F:1594:PRO:CG | 2.33 | 0.75 |
| 1:D:400:ILE:H | 1:D:400:ILE:HD12 | 1.50 | 0.75 |
| 1:D:606:THR:HG22 | 1:D:608:GLY:H | 1.50 | 0.75 |
| 1:A:606:THR:HG22 | 1:A:608:GLY:H | 1.50 | 0.75 |
| 3:C:1365:GLU:C | 3:C:1366:ILE:CG1 | 2.54 | 0.75 |
| 3:F:1593:LYS:N | 3:F:1596:LEU:HD21 | 2.01 | 0.75 |
| 3:C:1396:LEU:HB3 | 3:C:1412:LEU:HD12 | 1.62 | 0.75 |
| 3:C:1376:ALA:CB | 3:C:1429:VAL:HG22 | 2.12 | 0.75 |
| 3:C:1389:PHE:CZ | 3:C:1443:GLN:CB | 2.54 | 0.75 |
| 3:C:1481:ASN:ND2 | 3:C:1567:LYS:HE3 | 2.00 | 0.75 |
| 4:G:48:MET:O | 4:G:52:ARG:HG3 | 1.87 | 0.75 |
| 3:C:1495:ASN:O | 3:C:1496:CYS:HB2 | 1.83 | 0.75 |
| 3:C:1497:PHE:CE2 | 3:C:1571:ALA:HB1 | 2.22 | 0.75 |
| 2:E:836:GLN:NE2 | 2:E:897:HIS:HE1 | 1.84 | 0.75 |
| 4:H:48:MET:O | 4:H:52:ARG:HG3 | 1.87 | 0.75 |
| 1:A:400:ILE:HD12 | 1:A:400:ILE:H | 1.50 | 0.75 |
| 3:C:1341:LEU:HD13 | 3:C:1368:THR:HB | 1.68 | 0.75 |
| 3:C:1481:ASN:HD22 | 3:C:1567:LYS:HE3 | 1.51 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:1396:LEU:O | 3:F:1399:LEU:HB2 | 1.87 | 0.75 |
| 4:H:18:ALA:N | 4:H:65:MET:HE3 | 2.02 | 0.75 |
| 3:C:1465:GLU:CG | 3:C:1465:GLU:O | 2.32 | 0.74 |
| 2:E:738:ASN:HB3 | 4:H:47:MET:SD | 2.26 | 0.74 |
| 3:F:1342:LYS:HB2 | 3:F:1367:CYS:HB2 | 1.69 | 0.74 |
| 1:A:253:ILE:CD1 | 1:A:289:VAL:HG13 | 2.06 | 0.74 |
| 2:B:836:GLN:H | 2:B:868:PRO:HG3 | 1.52 | 0.74 |
| 3:C:1485:ARG:O | 3:C:1486:ASP:HB2 | 1.86 | 0.74 |
| 1:A:372:GLU:CA | 1:A:373:ASP:CB | 2.65 | 0.74 |
| 1:A:487:GLU:H | 1:A:490:GLN:NE2 | 1.85 | 0.74 |
| 3:C:1450:ILE:HG22 | 3:C:1451:GLN:N | 2.02 | 0.74 |
| 3:C:1380:ILE:HD12 | 3:C:1380:ILE:N | 2.01 | 0.74 |
| 3:F:1450:ILE:O | 3:F:1450:ILE:HD12 | 1.87 | 0.74 |
| 3:F:1472:HIS:ND1 | 3:F:1473:PRO:HD2 | 2.02 | 0.74 |
| 3:C:1345:ILE:HD12 | 3:C:1363:ILE:O | 1.88 | 0.73 |
| 2:E:734:ILE:HG12 | 4:H:51:TYR:CD1 | 2.22 | 0.73 |
| 1:D:268:ARG:HB2 | 3:F:1378:MET:CE | 2.18 | 0.73 |
| 1:D:487:GLU:H | 1:D:490:GLN:NE2 | 1.85 | 0.73 |
| 3:F:1344:THR:HG21 | 3:F:1346:LYS:HE2 | 1.69 | 0.73 |
| 3:C:1361:THR:CB | 3:C:1442:HIS:ND1 | 2.52 | 0.73 |
| 3:C:1366:ILE:O | 3:C:1436:CYS:SG | 2.46 | 0.73 |
| 1:D:372:GLU:HA | 1:D:373:ASP:HB2 | 1.66 | 0.73 |
| 3:C:1481:ASN:HB2 | 3:C:1492:ALA:O | 1.87 | 0.73 |
| 1:D:84:VAL:HG13 | 1:D:101:VAL:HG21 | 1.69 | 0.73 |
| 2:E:836:GLN:H | 2:E:868:PRO:HG3 | 1.53 | 0.73 |
| 3:C:1426:LEU:HD13 | 3:C:1426:LEU:N | 2.03 | 0.73 |
| 2:E:819:ARG:HH11 | 2:E:819:ARG:CG | 2.01 | 0.73 |
| 3:F:1340:ASP:O | 3:F:1368:THR:HA | 1.89 | 0.73 |
| 1:D:20:MET:HE1 | 1:D:35:VAL:HG13 | 1.71 | 0.73 |
| 1:D:253:ILE:HD12 | 1:D:302:LEU:HD21 | 1.70 | 0.73 |
| 1:D:564:GLU:HG2 | 2:E:766:THR:HG23 | 1.71 | 0.72 |
| 3:C:1381:LEU:HA | 3:C:1456:LYS:O | 1.87 | 0.72 |
| 3:C:1443:GLN:O | 3:C:1443:GLN:CG | 2.38 | 0.72 |
| 1:D:541:LEU:CD1 | 2:E:786:SER:HB3 | 2.20 | 0.72 |
| 3:F:1389:PHE:O | 3:F:1444:TYR:HE2 | 1.71 | 0.72 |
| 1:A:84:VAL:HG13 | 1:A:101:VAL:HG21 | 1.69 | 0.72 |
| 3:C:1390:ALA:CB | 3:C:1416:PHE:HD1 | 2.02 | 0.72 |
| 3:C:1403:VAL:HG22 | 3:C:1404:ASP:OD1 | 1.90 | 0.72 |
| 3:C:1592:GLU:OE1 | 3:C:1592:GLU:HA | 1.89 | 0.72 |
| 1:D:253:ILE:HD13 | 1:D:302:LEU:HD23 | 1.69 | 0.72 |
| 1:A:253:ILE:HD13 | 1:A:289:VAL:HG11 | 1.72 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:641:PRO:O | 1:A:642:GLN:HB2 | 1.90 | 0.72 |
| 3:F:1422:LEU:HD23 | 3:F:1422:LEU:O | 1.90 | 0.72 |
| 1:A:20:MET:HE1 | 1:A:35:VAL:HG13 | 1.70 | 0.72 |
| 3:C:1507:LEU:O | 3:C:1507:LEU:HD22 | 1.90 | 0.71 |
| 2:B:819:ARG:HD2 | 2:B:881:LEU:O | 1.90 | 0.71 |
| 1:A:183:LYS:HZ1 | 1:A:185:ARG:HD2 | 1.54 | 0.71 |
| 3:C:1520:ASP:OD1 | 3:C:1550:GLY:HA3 | 1.90 | 0.71 |
| 1:D:291:ASN:O | 1:D:292:PRO:C | 2.27 | 0.71 |
| 3:F:1537:ASP:OD2 | 3:F:1569:ARG:HD2 | 1.90 | 0.71 |
| 3:C:1337:ASN:O | 3:C:1371:ARG:HD3 | 1.90 | 0.71 |
| 3:C:1537:ASP:OD2 | 3:C:1569:ARG:HD2 | 1.90 | 0.71 |
| 3:F:1520:ASP:OD1 | 3:F:1550:GLY:HA3 | 1.90 | 0.71 |
| 2:E:845:LEU:HD21 | 2:E:891:LYS:HE3 | 1.72 | 0.71 |
| 3:F:1417:SER:OG | 3:F:1418:ASP:N | 2.19 | 0.71 |
| 4:G:75:ILE:O | 4:G:79:ILE:HG13 | 1.90 | 0.71 |
| 4:H:75:ILE:O | 4:H:79:ILE:HG13 | 1.90 | 0.71 |
| 1:A:345:GLY:N | 1:A:392:HIS:O | 2.24 | 0.71 |
| 3:C:1497:PHE:HE2 | 3:C:1571:ALA:HB1 | 1.56 | 0.71 |
| 1:D:370:GLN:HG2 | 1:D:401:THR:HB | 1.73 | 0.71 |
| 2:E:756:LEU:HA | 2:E:758:GLU:OE1 | 1.91 | 0.71 |
| 3:F:1393:THR:HG23 | 3:F:1419:ARG:HH12 | 1.56 | 0.71 |
| 3:C:1365:GLU:C | 3:C:1366:ILE:HG12 | 2.09 | 0.71 |
| 3:C:1543:ILE:HD12 | 3:C:1554:VAL:CG2 | 2.20 | 0.71 |
| 3:F:1507:LEU:HD22 | 3:F:1507:LEU:O | 1.90 | 0.71 |
| 3:C:1390:ALA:HB3 | 3:C:1416:PHE:HD1 | 1.47 | 0.71 |
| 3:C:1488:LEU:CD2 | 3:C:1590:TRP:CH2 | 2.74 | 0.71 |
| 1:D:641:PRO:O | 1:D:642:GLN:HB2 | 1.90 | 0.71 |
| 2:E:819:ARG:HD2 | 2:E:881:LEU:O | 1.91 | 0.71 |
| 2:E:820:ASN:ND2 | 3:F:1489:CYS:HB2 | 2.06 | 0.71 |
| 3:C:1379:SER:CA | 3:C:1380:ILE:HD12 | 2.21 | 0.70 |
| 1:D:253:ILE:HD12 | 1:D:302:LEU:CD2 | 2.16 | 0.70 |
| 3:F:1592:GLU:HA | 3:F:1592:GLU:OE1 | 1.89 | 0.70 |
| 1:A:370:GLN:HG2 | 1:A:401:THR:HB | 1.73 | 0.70 |
| 3:F:1591:GLY:C | 3:F:1596:LEU:HB3 | 2.09 | 0.70 |
| 1:A:292:PRO:HB3 | 3:F:1553:GLU:CB | 2.21 | 0.70 |
| 1:A:48:SER:O | 1:A:49:SER:O | 2.09 | 0.70 |
| 1:A:567:HIS:CE1 | 2:B:760:PRO:HD3 | 2.26 | 0.70 |
| 2:E:734:ILE:HA | 4:H:51:TYR:CE1 | 2.25 | 0.70 |
| 2:B:819:ARG:HH11 | 2:B:819:ARG:CG | 2.04 | 0.70 |
| 2:E:734:ILE:HD12 | 2:E:900:SER:HB3 | 1.74 | 0.70 |
| 1:A:332:GLN:HE21 | 1:A:357:PRO:HA | 1.57 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:1481:ASN:ND2 | 3:C:1567:LYS:CE | 2.54 | 0.70 |
| 1:D:207:LEU:HD21 | 2:E:747:GLU:HG2 | 1.73 | 0.70 |
| 2:B:910:VAL:HG22 | 2:B:911:PRO:HD2 | 1.73 | 0.69 |
| 3:F:1480:LEU:O | 3:F:1481:ASN:CG | 2.29 | 0.69 |
| 3:F:1592:GLU:HA | 3:F:1596:LEU:HD23 | 1.74 | 0.69 |
| 1:A:290:GLN:O | 1:A:290:GLN:CG | 2.41 | 0.69 |
| 1:D:372:GLU:CA | 1:D:373:ASP:CB | 2.65 | 0.69 |
| 3:F:1572:LEU:HD22 | 3:F:1574:LEU:HD21 | 1.75 | 0.69 |
| 1:D:253:ILE:CD1 | 1:D:302:LEU:HD23 | 2.18 | 0.69 |
| 3:F:1567:LYS:O | 3:F:1567:LYS:HG3 | 1.93 | 0.69 |
| 1:D:69:PRO:HA | 1:D:70:ALA:CB | 2.22 | 0.69 |
| 1:A:291:ASN:HB3 | 1:A:292:PRO:HD2 | 1.74 | 0.69 |
| 3:C:1389:PHE:CD1 | 3:C:1443:GLN:N | 2.60 | 0.69 |
| 3:C:1450:ILE:CG2 | 3:C:1451:GLN:N | 2.56 | 0.69 |
| 1:D:154:LYS:HD2 | 1:D:171:TRP:CD1 | 2.27 | 0.69 |
| 1:A:114:LYS:HE3 | 1:A:116:ILE:O | 1.92 | 0.69 |
| 2:B:734:ILE:HD12 | 2:B:900:SER:HB3 | 1.74 | 0.69 |
| 2:B:847:ASN:OD1 | 2:B:848:PRO:HD2 | 1.92 | 0.69 |
| 1:D:48:SER:O | 1:D:49:SER:O | 2.09 | 0.69 |
| 3:F:1387:THR:HG23 | 3:F:1451:GLN:H | 1.57 | 0.69 |
| 1:D:332:GLN:HE21 | 1:D:357:PRO:HA | 1.57 | 0.69 |
| 3:F:1462:ASN:HD22 | 3:F:1464:GLU:H | 1.41 | 0.69 |
| 1:A:69:PRO:HA | 1:A:70:ALA:CB | 2.22 | 0.68 |
| 1:A:154:LYS:HD2 | 1:A:171:TRP:CD1 | 2.27 | 0.68 |
| 3:C:1497:PHE:CD1 | 3:C:1498:ILE:O | 2.46 | 0.68 |
| 3:C:1543:ILE:CD1 | 3:C:1554:VAL:HG21 | 2.23 | 0.68 |
| 1:D:114:LYS:HE3 | 1:D:116:ILE:O | 1.92 | 0.68 |
| 2:E:758:GLU:HG2 | 2:E:765:SER:HB2 | 1.76 | 0.68 |
| 3:F:1407:ILE:CD1 | 3:F:1424:ILE:HG12 | 2.24 | 0.68 |
| 3:C:1344:THR:HG21 | 3:C:1346:LYS:HE2 | 1.74 | 0.68 |
| 3:C:1567:LYS:HG3 | 3:C:1567:LYS:O | 1.93 | 0.68 |
| 3:F:1405:ARG:HD3 | 3:F:1426:LEU:CD2 | 2.24 | 0.68 |
| 1:A:104:GLN:O | 1:A:132:HIS:CE1 | 2.46 | 0.68 |
| 1:A:292:PRO:HD2 | 1:A:296:ASP:OD2 | 1.93 | 0.68 |
| 3:C:1581:LEU:HD12 | 3:C:1582:MET:N | 2.09 | 0.68 |
| 3:F:1341:LEU:HD21 | 3:F:1455:VAL:CG1 | 2.22 | 0.67 |
| 3:F:1498:ILE:O | 3:F:1499:GLN:O | 2.12 | 0.67 |
| 3:F:1581:LEU:HD12 | 3:F:1582:MET:N | 2.09 | 0.67 |
| 2:B:845:LEU:HD21 | 2:B:891:LYS:HE3 | 1.76 | 0.67 |
| 2:B:887:GLU:HB2 | 2:B:906:SER:OG | 1.94 | 0.67 |
| 3:C:1365:GLU:CG | 3:C:1366:ILE:H | 2.08 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:910:VAL:HG22 | 2:E:911:PRO:HD2 | 1.75 | 0.67 |
| 1:A:69:PRO:CA | 1:A:70:ALA:HB3 | 2.25 | 0.67 |
| 1:A:126:ARG:NH2 | 1:A:573:LEU:O | 2.28 | 0.67 |
| 1:A:438:VAL:HG23 | 1:A:450:ASN:O | 1.95 | 0.67 |
| 3:C:1389:PHE:CG | 3:C:1443:GLN:CB | 2.70 | 0.67 |
| 3:C:1572:LEU:HD22 | 3:C:1574:LEU:HD21 | 1.75 | 0.67 |
| 3:F:1397:LYS:HD3 | 3:F:1397:LYS:N | 2.10 | 0.67 |
| 1:A:236:ARG:HA | 1:A:243:VAL:HG23 | 1.77 | 0.67 |
| 3:C:1617:ASP:HB2 | 3:C:1620:ASN:HB2 | 1.77 | 0.67 |
| 2:E:746:PRO:HG3 | 2:E:774:LYS:HD2 | 1.75 | 0.67 |
| 2:E:847:ASN:OD1 | 2:E:848:PRO:HD2 | 1.95 | 0.67 |
| 1:D:204:GLU:HG2 | 2:E:815:TYR:CE2 | 2.30 | 0.67 |
| 3:C:1426:LEU:CD1 | 3:C:1426:LEU:N | 2.58 | 0.67 |
| 3:F:1341:LEU:HD22 | 3:F:1457:VAL:HG22 | 1.75 | 0.67 |
| 1:D:126:ARG:NH2 | 1:D:573:LEU:O | 2.28 | 0.67 |
| 2:E:738:ASN:O | 4:H:47:MET:CE | 2.42 | 0.67 |
| 3:F:1347:PRO:HA | 3:F:1362:MET:HG2 | 1.76 | 0.67 |
| 1:D:104:GLN:O | 1:D:132:HIS:CE1 | 2.46 | 0.66 |
| 1:D:438:VAL:HG23 | 1:D:450:ASN:O | 1.95 | 0.66 |
| 4:H:18:ALA:N | 4:H:65:MET:CE | 2.58 | 0.66 |
| 3:F:1404:ASP:HA | 3:F:1427:ASP:HB2 | 1.76 | 0.66 |
| 1:A:6:ILE:CD1 | 1:A:22:LEU:HD23 | 2.26 | 0.66 |
| 3:C:1386:MET:SD | 3:C:1473:PRO:HD3 | 2.36 | 0.66 |
| 1:D:364:ARG:N | 1:D:379:THR:HG22 | 2.10 | 0.66 |
| 3:F:1403:VAL:HG22 | 3:F:1404:ASP:CG | 2.15 | 0.66 |
| 3:F:1483:LEU:HD21 | 3:F:1590:TRP:CD2 | 2.30 | 0.66 |
| 1:D:69:PRO:CA | 1:D:70:ALA:HB3 | 2.25 | 0.66 |
| 3:F:1411:GLU:O | 3:F:1413:ASP:N | 2.27 | 0.66 |
| 3:F:1399:LEU:HD23 | 3:F:1405:ARG:NH1 | 2.10 | 0.66 |
| 1:D:236:ARG:HA | 1:D:243:VAL:HG23 | 1.77 | 0.66 |
| 2:B:746:PRO:HG3 | 2:B:774:LYS:HD2 | 1.78 | 0.66 |
| 1:A:364:ARG:N | 1:A:379:THR:HG22 | 2.10 | 0.65 |
| 1:D:6:ILE:CD1 | 1:D:22:LEU:HD23 | 2.26 | 0.65 |
| 1:A:530:TRP:CH2 | 1:A:532:ASP:HB2 | 2.31 | 0.65 |
| 3:F:1407:ILE:HD11 | 3:F:1424:ILE:CG1 | 2.25 | 0.65 |
| 3:F:1614:GLU:O | 3:F:1620:ASN:HB2 | 1.96 | 0.65 |
| 3:F:1345:ILE:HD12 | 3:F:1363:ILE:O | 1.96 | 0.65 |
| 1:A:400:ILE:HD13 | 1:A:419:MET:HE3 | 1.79 | 0.65 |
| 1:A:547:GLN:OE1 | 1:A:559:MET:HA | 1.96 | 0.65 |
| 3:C:1390:ALA:O | 3:C:1416:PHE:HE1 | 1.79 | 0.65 |
| 2:B:836:GLN:HE21 | 2:B:897:HIS:HE1 | 1.42 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:1365:GLU:CG | 3:C:1366:ILE:N | 2.59 | 0.65 |
| 3:C:1381:LEU:CD1 | 3:C:1383:ILE:HD11 | 2.20 | 0.65 |
| 3:C:1462:ASN:HD21 | 3:C:1464:GLU:HB2 | 1.60 | 0.65 |
| 3:C:1495:ASN:HD22 | 3:C:1496:CYS:H | 1.45 | 0.65 |
| 1:D:22:LEU:HD22 | 1:D:33:VAL:HG11 | 1.79 | 0.65 |
| 2:B:756:LEU:HA | 2:B:758:GLU:OE1 | 1.96 | 0.64 |
| 2:B:856:THR:H | 3:C:1602:LYS:HZ2 | 1.44 | 0.64 |
| 1:A:372:GLU:HA | 1:A:373:ASP:HB2 | 1.66 | 0.64 |
| 1:A:455:LEU:HD11 | 1:A:457:MET:HG2 | 1.78 | 0.64 |
| 1:D:183:LYS:HZ1 | 1:D:185:ARG:HD2 | 1.61 | 0.64 |
| 1:A:22:LEU:HD22 | 1:A:33:VAL:HG11 | 1.79 | 0.64 |
| 1:D:400:ILE:HD13 | 1:D:419:MET:HE3 | 1.78 | 0.64 |
| 1:D:455:LEU:HD11 | 1:D:457:MET:HG2 | 1.78 | 0.64 |
| 1:D:530:TRP:CH2 | 1:D:532:ASP:HB2 | 2.31 | 0.64 |
| 1:D:116:ILE:HG13 | 1:D:201:GLU:HB3 | 1.79 | 0.64 |
| 3:F:1335:THR:O | 3:F:1336:CYS:HB2 | 1.97 | 0.64 |
| 1:D:370:GLN:HA | 1:D:370:GLN:OE1 | 1.98 | 0.64 |
| 3:F:1415:ALA:C | 3:F:1417:SER:H | 1.99 | 0.64 |
| 3:F:1616:GLN:N | 3:F:1616:GLN:OE1 | 2.30 | 0.64 |
| 4:G:77:LYS:O | 4:G:81:GLU:HG3 | 1.98 | 0.64 |
| 1:A:183:LYS:NZ | 1:A:185:ARG:HD2 | 2.12 | 0.64 |
| 3:C:1389:PHE:CD1 | 3:C:1441:VAL:HG23 | 2.33 | 0.64 |
| 3:C:1424:ILE:HG22 | 3:C:1426:LEU:HD11 | 1.79 | 0.64 |
| 1:D:6:ILE:HG12 | 1:D:20:MET:HE3 | 1.80 | 0.64 |
| 1:D:183:LYS:NZ | 1:D:185:ARG:HD2 | 2.12 | 0.64 |
| 1:A:116:ILE:HG13 | 1:A:201:GLU:HB3 | 1.79 | 0.64 |
| 1:A:6:ILE:HG22 | 1:A:625:THR:HB | 1.80 | 0.64 |
| 3:F:1593:LYS:CA | 3:F:1596:LEU:HD21 | 2.28 | 0.64 |
| 2:E:860:HIS:HE1 | 3:F:1451:GLN:HE21 | 1.44 | 0.63 |
| 3:F:1561:THR:O | 3:F:1597:SER:HB3 | 1.98 | 0.63 |
| 3:C:1361:THR:CG2 | 3:C:1442:HIS:ND1 | 2.61 | 0.63 |
| 1:A:370:GLN:OE1 | 1:A:370:GLN:HA | 1.98 | 0.63 |
| 3:F:1483:LEU:HD21 | 3:F:1590:TRP:NE1 | 2.13 | 0.63 |
| 3:C:1546:THR:HG23 | 3:C:1556:VAL:HG22 | 1.80 | 0.63 |
| 3:F:1608:HIS:O | 3:F:1610:PRO:HD3 | 1.99 | 0.63 |
| 4:H:77:LYS:O | 4:H:81:GLU:HG3 | 1.98 | 0.63 |
| 3:C:1415:ALA:H | 3:C:1419:ARG:NH2 | 1.96 | 0.63 |
| 2:E:820:ASN:HD21 | 3:F:1489:CYS:HB2 | 1.64 | 0.63 |
| 2:E:836:GLN:HE21 | 2:E:897:HIS:HE1 | 1.47 | 0.63 |
| 1:A:6:ILE:HG12 | 1:A:20:MET:HE3 | 1.81 | 0.63 |
| 1:D:31:VAL:HG13 | 1:D:54:LEU:HB2 | 1.81 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:E:898:PHE:HB2 | 4:H:52:ARG:HG2 | 1.80 | 0.63 |
| 1:A:31:VAL:HG13 | 1:A:54:LEU:HB2 | 1.81 | 0.62 |
| 3:C:1389:PHE:CE2 | 3:C:1443:GLN:HB3 | 2.04 | 0.62 |
| 3:C:1481:ASN:HD22 | 3:C:1567:LYS:CE | 2.11 | 0.62 |
| 3:F:1456:LYS:HA | 3:F:1467:CYS:O | 2.00 | 0.62 |
| 3:C:1404:ASP:CA | 3:C:1427:ASP:CG | 2.62 | 0.62 |
| 1:D:590:THR:HB | 1:D:593:LYS:HG3 | 1.82 | 0.62 |
| 3:C:1344:THR:CG2 | 3:C:1346:LYS:HE2 | 2.30 | 0.62 |
| 1:D:6:ILE:HG22 | 1:D:625:THR:HB | 1.80 | 0.62 |
| 1:D:36:THR:HG21 | 1:D:38:HIS:CE1 | 2.35 | 0.62 |
| 2:E:761:LYS:O | 2:E:762:ASN:CB | 2.47 | 0.62 |
| 3:F:1346:LYS:O | 3:F:1362:MET:HB3 | 1.99 | 0.62 |
| 1:A:36:THR:HG21 | 1:A:38:HIS:CE1 | 2.35 | 0.62 |
| 3:F:1342:LYS:HE2 | 3:F:1434:ASP:OD2 | 1.98 | 0.62 |
| 3:F:1483:LEU:HD11 | 3:F:1590:TRP:NE1 | 2.15 | 0.62 |
| 3:C:1390:ALA:HB3 | 3:C:1416:PHE:CE1 | 2.35 | 0.62 |
| 3:C:1608:HIS:O | 3:C:1610:PRO:HD3 | 1.99 | 0.62 |
| 2:B:836:GLN:NE2 | 2:B:897:HIS:CE1 | 2.67 | 0.62 |
| 2:E:887:GLU:HB2 | 2:E:906:SER:OG | 2.00 | 0.62 |
| 3:C:1387:THR:HG23 | 3:C:1451:GLN:HB3 | 1.80 | 0.62 |
| 1:D:268:ARG:HB2 | 3:F:1378:MET:HE2 | 1.81 | 0.62 |
| 3:C:1475:LYS:NZ | 3:C:1493:GLU:OE2 | 2.32 | 0.61 |
| 3:C:1337:ASN:HB2 | 3:C:1338:LYS:HD2 | 1.82 | 0.61 |
| 4:H:61:ASP:HB3 | 4:H:64:SER:OG | 1.99 | 0.61 |
| 1:A:590:THR:HB | 1:A:593:LYS:HG3 | 1.82 | 0.61 |
| 2:B:734:ILE:HA | 4:G:51:TYR:CE1 | 2.34 | 0.61 |
| 1:D:541:LEU:HD13 | 2:E:786:SER:CB | 2.29 | 0.61 |
| 2:E:894:VAL:CG1 | 2:E:899:ILE:HB | 2.30 | 0.61 |
| 3:F:1521:TYR:CZ | 3:F:1584:GLY:N | 2.68 | 0.61 |
| 3:F:1614:GLU:HB3 | 3:F:1620:ASN:ND2 | 2.16 | 0.61 |
| 3:C:1464:GLU:OE1 | 3:C:1464:GLU:N | 2.30 | 0.61 |
| 1:D:590:THR:HG22 | 1:D:592:SER:H | 1.65 | 0.61 |
| 3:F:1371:ARG:NH1 | 3:F:1371:ARG:HG2 | 2.14 | 0.61 |
| 1:D:297:LEU:HA | 1:D:300:LYS:HD2 | 1.82 | 0.61 |
| 3:C:1379:SER:O | 3:C:1380:ILE:CD1 | 2.44 | 0.61 |
| 3:C:1389:PHE:CA | 3:C:1443:GLN:HA | 2.31 | 0.61 |
| 3:F:1456:LYS:HE2 | 3:F:1458:TYR:CD2 | 2.36 | 0.61 |
| 3:F:1462:ASN:ND2 | 3:F:1464:GLU:N | 2.48 | 0.61 |
| 3:F:1483:LEU:HD11 | 3:F:1590:TRP:HE1 | 1.65 | 0.61 |
| 3:C:1544:GLU:C | 3:C:1556:VAL:CG1 | 2.69 | 0.61 |
| 1:A:606:THR:HG22 | 1:A:608:GLY:N | 2.16 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:1453:GLY:HA3 | 3:C:1471:TYR:CZ | 2.36 | 0.61 |
| 1:D:606:THR:HG22 | 1:D:608:GLY:N | 2.16 | 0.61 |
| 3:F:1480:LEU:O | 3:F:1481:ASN:ND2 | 2.34 | 0.61 |
| 3:C:1361:THR:HA | 3:C:1441:VAL:O | 2.01 | 0.60 |
| 3:C:1406:TYR:CE1 | 3:C:1408:SER:HA | 2.36 | 0.60 |
| 3:C:1521:TYR:CZ | 3:C:1584:GLY:N | 2.68 | 0.60 |
| 1:A:297:LEU:HA | 1:A:300:LYS:HD2 | 1.82 | 0.60 |
| 3:C:1366:ILE:C | 3:C:1367:CYS:SG | 2.76 | 0.60 |
| 1:D:142:MET:HG3 | 1:D:187:TYR:CE1 | 2.36 | 0.60 |
| 2:E:819:ARG:HG2 | 2:E:819:ARG:NH1 | 2.13 | 0.60 |
| 2:E:845:LEU:HD22 | 2:E:889:GLU:HG2 | 1.83 | 0.60 |
| 1:A:346:MET:HE2 | 1:A:456:ARG:HB2 | 1.82 | 0.60 |
| 3:C:1339:PHE:CZ | 3:C:1370:TYR:CD1 | 2.89 | 0.60 |
| 1:D:268:ARG:HB2 | 3:F:1378:MET:HE1 | 1.82 | 0.60 |
| 3:F:1405:ARG:HD3 | 3:F:1426:LEU:HD23 | 1.83 | 0.60 |
| 1:A:36:THR:CG2 | 1:A:38:HIS:CE1 | 2.85 | 0.60 |
| 3:C:1361:THR:HB | 3:C:1442:HIS:CE1 | 2.37 | 0.60 |
| 3:C:1408:SER:C | 3:C:1410:TYR:H | 2.04 | 0.60 |
| 1:A:590:THR:HG22 | 1:A:592:SER:H | 1.65 | 0.60 |
| 1:A:606:THR:HB | 1:A:619:ASP:HB3 | 1.84 | 0.60 |
| 3:C:1416:PHE:O | 3:C:1417:SER:C | 2.39 | 0.60 |
| 3:F:1495:ASN:O | 3:F:1496:CYS:C | 2.39 | 0.60 |
| 1:D:36:THR:CG2 | 1:D:38:HIS:CE1 | 2.85 | 0.60 |
| 1:A:142:MET:HG3 | 1:A:187:TYR:CE1 | 2.36 | 0.60 |
| 2:E:872:LEU:HD11 | 3:F:1418:ASP:HB3 | 1.83 | 0.60 |
| 3:F:1404:ASP:HB3 | 3:F:1427:ASP:HB2 | 1.83 | 0.60 |
| 3:F:1504:LYS:O | 3:F:1505:VAL:CG2 | 2.45 | 0.60 |
| 3:C:1388:GLY:O | 3:C:1443:GLN:HA | 2.01 | 0.59 |
| 3:C:1543:ILE:O | 3:C:1557:GLY:N | 2.35 | 0.59 |
| 3:C:1544:GLU:O | 3:C:1556:VAL:CG1 | 2.50 | 0.59 |
| 2:E:764:ILE:O | 2:E:764:ILE:CG2 | 2.44 | 0.59 |
| 3:F:1490:ARG:HD2 | 3:F:1590:TRP:CZ3 | 2.37 | 0.59 |
| 1:A:241:LYS:HG3 | 2:B:832:TYR:CZ | 2.37 | 0.59 |
| 3:C:1368:THR:HG21 | 3:C:1457:VAL:HG11 | 1.84 | 0.59 |
| 4:H:45:THR:HG21 | 4:H:75:ILE:HD13 | 1.84 | 0.59 |
| 3:C:1444:TYR:O | 3:C:1445:PHE:HB3 | 2.02 | 0.59 |
| 3:C:1386:MET:HB3 | 3:C:1450:ILE:HG21 | 1.84 | 0.59 |
| 1:D:606:THR:HB | 1:D:619:ASP:HB3 | 1.84 | 0.59 |
| 2:B:834:GLN:HE21 | 2:B:834:GLN:HA | 1.68 | 0.59 |
| 3:C:1458:TYR:HB3 | 3:C:1466:SER:HB3 | 1.84 | 0.59 |
| 3:C:1472:HIS:HB3 | 3:C:1475:LYS:HB2 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:471:LEU:N | 1:D:471:LEU:HD12 | 2.17 | 0.59 |
| 3:F:1380:ILE:O | 3:F:1457:VAL:HG12 | 2.03 | 0.59 |
| 3:C:1450:ILE:CG2 | 3:C:1451:GLN:H | 2.16 | 0.59 |
| 3:C:1504:LYS:O | 3:C:1505:VAL:CG2 | 2.45 | 0.59 |
| 1:D:290:GLN:O | 1:D:290:GLN:CG | 2.49 | 0.59 |
| 3:F:1345:ILE:HG23 | 3:F:1345:ILE:O | 2.01 | 0.59 |
| 2:B:894:VAL:CG1 | 2:B:899:ILE:HB | 2.32 | 0.59 |
| 3:C:1433:GLU:O | 3:C:1434:ASP:CB | 2.51 | 0.59 |
| 1:D:257:GLU:N | 1:D:257:GLU:OE2 | 2.36 | 0.59 |
| 1:D:550:ASP:O | 1:D:551:ARG:C | 2.39 | 0.59 |
| 2:E:860:HIS:CE1 | 3:F:1451:GLN:HE21 | 2.21 | 0.59 |
| 3:C:1454:ALA:HB2 | 3:C:1470:PHE:CD2 | 2.38 | 0.58 |
| 1:D:143:VAL:O | 1:D:155:GLN:HB2 | 2.03 | 0.58 |
| 3:F:1380:ILE:O | 3:F:1457:VAL:HA | 2.02 | 0.58 |
| 3:F:1389:PHE:O | 3:F:1444:TYR:CE2 | 2.55 | 0.58 |
| 3:F:1407:ILE:HG22 | 3:F:1412:LEU:HD22 | 1.85 | 0.58 |
| 3:F:1482:LYS:O | 3:F:1482:LYS:HG2 | 2.02 | 0.58 |
| 1:D:282:ARG:HH12 | 1:D:286:LEU:HD12 | 1.68 | 0.58 |
| 3:F:1456:LYS:HE2 | 3:F:1458:TYR:HD2 | 1.67 | 0.58 |
| 4:G:45:THR:HG21 | 4:G:75:ILE:HD13 | 1.84 | 0.58 |
| 1:A:477:ARG:HG3 | 1:A:477:ARG:HH11 | 1.68 | 0.58 |
| 1:D:346:MET:HG2 | 1:D:347:PRO:HD2 | 1.86 | 0.58 |
| 1:A:471:LEU:N | 1:A:471:LEU:HD12 | 2.17 | 0.58 |
| 1:A:472:ILE:HD13 | 1:A:509:LEU:HD22 | 1.85 | 0.58 |
| 3:C:1397:LYS:HA | 3:C:1400:ALA:HB3 | 1.84 | 0.58 |
| 1:D:6:ILE:HD11 | 1:D:20:MET:CG | 2.34 | 0.58 |
| 1:D:291:ASN:HB3 | 1:D:292:PRO:HD2 | 1.86 | 0.58 |
| 3:F:1383:ILE:HG12 | 3:F:1455:VAL:HG22 | 1.85 | 0.58 |
| 2:B:845:LEU:HD22 | 2:B:889:GLU:HG2 | 1.85 | 0.58 |
| 3:C:1338:LYS:CD | 3:C:1465:GLU:HB2 | 2.34 | 0.58 |
| 4:H:18:ALA:HB3 | 4:H:20:GLU:HG2 | 1.86 | 0.58 |
| 3:C:1380:ILE:CG2 | 3:C:1423:ILE:HG23 | 2.32 | 0.58 |
| 3:C:1407:ILE:HD11 | 3:C:1424:ILE:HG12 | 1.85 | 0.58 |
| 3:F:1404:ASP:CA | 3:F:1427:ASP:HB2 | 2.33 | 0.58 |
| 2:E:738:ASN:O | 4:H:47:MET:HE1 | 2.03 | 0.58 |
| 1:D:472:ILE:HD13 | 1:D:509:LEU:HD22 | 1.85 | 0.58 |
| 1:D:477:ARG:HG3 | 1:D:477:ARG:HH11 | 1.68 | 0.58 |
| 3:F:1590:TRP:O | 3:F:1596:LEU:CA | 2.50 | 0.58 |
| 1:A:257:GLU:N | 1:A:257:GLU:OE2 | 2.36 | 0.57 |
| 1:D:204:GLU:OE1 | 2:E:815:TYR:HE2 | 1.87 | 0.57 |
| 3:F:1506:THR:OG1 | 3:F:1509:GLU:HG3 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:836:GLN:H | 2:B:868:PRO:CG | 2.16 | 0.57 |
| 3:C:1499:GLN:O | 3:C:1499:GLN:CD | 2.42 | 0.57 |
| 1:D:404:THR:CG2 | 1:D:415:ALA:H | 2.17 | 0.57 |
| 3:C:1506:THR:OG1 | 3:C:1509:GLU:HG3 | 2.04 | 0.57 |
| 1:D:67:THR:O | 1:D:69:PRO:HD3 | 2.05 | 0.57 |
| 3:F:1450:ILE:HD12 | 3:F:1450:ILE:C | 2.24 | 0.57 |
| 1:A:6:ILE:HD11 | 1:A:20:MET:CG | 2.34 | 0.57 |
| 1:A:330:PRO:HG2 | 1:A:409:LEU:HD21 | 1.86 | 0.57 |
| 1:A:346:MET:O | 1:A:347:PRO:O | 2.22 | 0.57 |
| 1:A:474:ASN:HB3 | 1:A:477:ARG:HH12 | 1.70 | 0.57 |
| 3:F:1365:GLU:HG3 | 3:F:1438:ALA:HB2 | 1.85 | 0.57 |
| 1:A:404:THR:CG2 | 1:A:415:ALA:H | 2.17 | 0.57 |
| 3:F:1381:LEU:HG | 3:F:1426:LEU:HD11 | 1.87 | 0.57 |
| 3:F:1497:PHE:HB3 | 3:F:1600:ILE:CG2 | 2.34 | 0.57 |
| 3:F:1623:GLN:O | 3:F:1627:LEU:HG | 2.04 | 0.57 |
| 4:G:18:ALA:HB3 | 4:G:20:GLU:HG2 | 1.86 | 0.57 |
| 1:A:67:THR:O | 1:A:69:PRO:HD3 | 2.05 | 0.57 |
| 3:F:1371:ARG:HG2 | 3:F:1371:ARG:HH11 | 1.70 | 0.57 |
| 1:A:282:ARG:HH12 | 1:A:286:LEU:HD12 | 1.68 | 0.57 |
| 3:C:1406:TYR:CZ | 3:C:1408:SER:HA | 2.39 | 0.57 |
| 3:C:1488:LEU:HG | 3:C:1489:CYS:H | 1.68 | 0.57 |
| 3:C:1380:ILE:O | 3:C:1457:VAL:HA | 2.05 | 0.57 |
| 1:D:330:PRO:HG2 | 1:D:409:LEU:HD21 | 1.86 | 0.57 |
| 1:D:438:VAL:HG22 | 1:D:449:LEU:HD11 | 1.86 | 0.57 |
| 2:E:761:LYS:O | 2:E:762:ASN:HB2 | 2.05 | 0.57 |
| 1:A:158:LEU:HD21 | 1:A:167:LEU:HD22 | 1.87 | 0.56 |
| 3:C:1472:HIS:CE1 | 3:C:1474:GLU:HG2 | 2.40 | 0.56 |
| 3:C:1563:ILE:HG12 | 3:C:1598:TYR:O | 2.05 | 0.56 |
| 1:D:158:LEU:HD21 | 1:D:167:LEU:HD22 | 1.87 | 0.56 |
| 1:D:251:PHE:CE1 | 1:D:304:VAL:HG13 | 2.40 | 0.56 |
| 3:F:1411:GLU:C | 3:F:1413:ASP:H | 2.06 | 0.56 |
| 1:A:567:HIS:HA | 2:B:765:SER:HB2 | 1.86 | 0.56 |
| 2:E:836:GLN:H | 2:E:868:PRO:CG | 2.17 | 0.56 |
| 3:F:1563:ILE:HG12 | 3:F:1598:TYR:O | 2.05 | 0.56 |
| 3:C:1443:GLN:HE21 | 3:C:1450:ILE:HD11 | 1.70 | 0.56 |
| 3:C:1630:PHE:O | 3:C:1634:MET:HG2 | 2.05 | 0.56 |
| 2:E:868:PRO:O | 2:E:869:LYS:C | 2.44 | 0.56 |
| 3:F:1384:SER:OG | 3:F:1454:ALA:HB3 | 2.05 | 0.56 |
| 3:C:1623:GLN:O | 3:C:1627:LEU:HG | 2.04 | 0.56 |
| 3:C:1376:ALA:CB | 3:C:1429:VAL:HG21 | 2.26 | 0.56 |
| 3:C:1437:LEU:HD12 | 3:C:1437:LEU:C | 2.24 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:1445:PHE:O | 3:C:1445:PHE:CD2 | 2.59 | 0.56 |
| 3:C:1465:GLU:O | 3:C:1465:GLU:HG2 | 2.05 | 0.56 |
| 1:D:335:PHE:CD1 | 1:D:419:MET:HG2 | 2.41 | 0.56 |
| 3:C:1476:GLU:O | 3:C:1478:GLY:N | 2.39 | 0.56 |
| 1:A:45:LEU:HD21 | 1:A:48:SER:CB | 2.35 | 0.56 |
| 1:A:456:ARG:HB2 | 1:A:456:ARG:HH11 | 1.70 | 0.56 |
| 3:F:1408:SER:O | 3:F:1410:TYR:N | 2.38 | 0.56 |
| 1:A:87:GLN:O | 1:A:87:GLN:HG2 | 2.05 | 0.56 |
| 3:C:1416:PHE:HZ | 3:C:1442:HIS:HB2 | 1.70 | 0.56 |
| 1:D:15:GLU:HG2 | 1:D:70:ALA:HB2 | 1.87 | 0.56 |
| 1:D:344:PRO:HA | 1:D:391:THR:HG21 | 1.86 | 0.56 |
| 3:F:1460:TYR:CG | 3:F:1461:TYR:N | 2.73 | 0.56 |
| 3:F:1630:PHE:O | 3:F:1634:MET:HG2 | 2.05 | 0.56 |
| 1:A:248:PHE:CD1 | 3:C:1378:MET:HE1 | 2.41 | 0.56 |
| 2:B:822:GLN:NE2 | 3:C:1470:PHE:CD1 | 2.72 | 0.56 |
| 1:A:15:GLU:HG2 | 1:A:70:ALA:HB2 | 1.87 | 0.56 |
| 1:A:136:PRO:CG | 2:B:789:ASP:HA | 2.36 | 0.56 |
| 1:D:456:ARG:HH11 | 1:D:456:ARG:HB2 | 1.70 | 0.56 |
| 1:D:474:ASN:HB3 | 1:D:477:ARG:HH12 | 1.70 | 0.56 |
| 3:F:1371:ARG:HH11 | 3:F:1371:ARG:CG | 2.17 | 0.56 |
| 3:F:1497:PHE:N | 3:F:1497:PHE:CD2 | 2.73 | 0.56 |
| 1:A:214:VAL:HB | 1:A:233:ILE:CD1 | 2.36 | 0.55 |
| 3:C:1404:ASP:O | 3:C:1405:ARG:HG2 | 2.06 | 0.55 |
| 2:E:756:LEU:CA | 2:E:758:GLU:OE1 | 2.53 | 0.55 |
| 1:A:251:PHE:CE1 | 1:A:304:VAL:HG13 | 2.40 | 0.55 |
| 1:A:541:LEU:HD13 | 2:B:786:SER:HB3 | 1.88 | 0.55 |
| 3:C:1499:GLN:O | 3:C:1500:LYS:C | 2.45 | 0.55 |
| 3:C:1465:GLU:O | 3:C:1465:GLU:HG3 | 2.04 | 0.55 |
| 1:D:45:LEU:HD21 | 1:D:48:SER:CB | 2.35 | 0.55 |
| 3:F:1389:PHE:HA | 3:F:1442:HIS:O | 2.06 | 0.55 |
| 1:A:142:MET:HG3 | 1:A:187:TYR:CZ | 2.41 | 0.55 |
| 1:A:438:VAL:HG22 | 1:A:449:LEU:HD11 | 1.86 | 0.55 |
| 1:D:142:MET:HG3 | 1:D:187:TYR:CZ | 2.41 | 0.55 |
| 3:F:1636:VAL:HG12 | 3:F:1637:PHE:CD2 | 2.42 | 0.55 |
| 1:D:87:GLN:HG2 | 1:D:87:GLN:O | 2.05 | 0.55 |
| 4:G:79:ILE:O | 4:G:83:ILE:HG12 | 2.07 | 0.55 |
| 4:H:65:MET:O | 4:H:68:ALA:N | 2.40 | 0.55 |
| 3:C:1397:LYS:HD3 | 3:C:1397:LYS:H | 1.72 | 0.55 |
| 3:F:1381:LEU:CD2 | 3:F:1457:VAL:CG1 | 2.81 | 0.55 |
| 4:H:79:ILE:O | 4:H:83:ILE:HG12 | 2.07 | 0.55 |
| 3:F:1462:ASN:ND2 | 3:F:1462:ASN:C | 2.56 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:335:PHE:CD1 | 1:A:419:MET:HG2 | 2.41 | 0.55 |
| 3:C:1377:THR:O | 3:C:1378:MET:C | 2.43 | 0.55 |
| 3:C:1636:VAL:HG12 | 3:C:1637:PHE:CD2 | 2.42 | 0.55 |
| 1:D:151:ILE:O | 1:D:153:VAL:HG13 | 2.07 | 0.55 |
| 1:D:214:VAL:HB | 1:D:233:ILE:CD1 | 2.36 | 0.55 |
| 1:D:552:GLN:HB3 | 1:D:553:PRO:CD | 2.32 | 0.55 |
| 3:C:1342:LYS:O | 3:C:1366:ILE:HA | 2.07 | 0.55 |
| 1:D:253:ILE:CD1 | 1:D:302:LEU:HD22 | 2.27 | 0.55 |
| 1:D:589:LEU:HD12 | 1:D:590:THR:H | 1.72 | 0.55 |
| 3:C:1408:SER:C | 3:C:1410:TYR:N | 2.59 | 0.54 |
| 3:F:1513:LYS:C | 3:F:1515:CYS:H | 2.10 | 0.54 |
| 1:A:548:SER:O | 1:A:549:GLU:HB3 | 2.07 | 0.54 |
| 2:B:851:CYS:HB2 | 2:B:881:LEU:HD21 | 1.88 | 0.54 |
| 3:C:1460:TYR:CG | 3:C:1461:TYR:N | 2.74 | 0.54 |
| 3:C:1566:ILE:C | 3:C:1568:CYS:H | 2.10 | 0.54 |
| 3:F:1364:LEU:HD21 | 3:F:1471:TYR:CZ | 2.43 | 0.54 |
| 3:F:1472:HIS:CD2 | 3:F:1475:LYS:HD2 | 2.42 | 0.54 |
| 1:A:549:GLU:CG | 1:A:550:ASP:H | 2.10 | 0.54 |
| 3:C:1340:ASP:O | 3:C:1368:THR:CA | 2.51 | 0.54 |
| 3:C:1380:ILE:HG22 | 3:C:1381:LEU:N | 2.22 | 0.54 |
| 3:C:1380:ILE:HG13 | 3:C:1425:TYR:CD1 | 2.41 | 0.54 |
| 3:C:1498:ILE:HG21 | 3:C:1605:TRP:CE3 | 2.42 | 0.54 |
| 3:F:1419:ARG:O | 3:F:1419:ARG:HG2 | 2.06 | 0.54 |
| 3:F:1566:ILE:HG13 | 3:F:1569:ARG:HD3 | 1.90 | 0.54 |
| 2:B:756:LEU:HD23 | 2:B:758:GLU:OE1 | 2.07 | 0.54 |
| 2:E:731:GLU:O | 2:E:732:ASP:HB2 | 2.07 | 0.54 |
| 1:A:151:ILE:O | 1:A:153:VAL:HG13 | 2.07 | 0.54 |
| 1:A:312:SER:HB2 | 1:A:314:SER:OG | 2.08 | 0.54 |
| 2:E:838:LEU:HD22 | 2:E:894:VAL:HG21 | 1.90 | 0.54 |
| 3:C:1380:ILE:CD1 | 3:C:1380:ILE:N | 2.67 | 0.54 |
| 1:A:550:ASP:OD2 | 1:A:551:ARG:N | 2.29 | 0.54 |
| 3:F:1566:ILE:C | 3:F:1568:CYS:H | 2.10 | 0.54 |
| 4:H:61:ASP:CG | 4:H:64:SER:OG | 2.46 | 0.54 |
| 1:A:589:LEU:HD12 | 1:A:590:THR:H | 1.72 | 0.54 |
| 3:C:1380:ILE:HG21 | 3:C:1423:ILE:HG21 | 1.84 | 0.54 |
| 1:D:517:GLY:O | 1:D:518:ALA:C | 2.46 | 0.54 |
| 1:A:454:LEU:CD2 | 1:A:492:LEU:CD1 | 2.81 | 0.54 |
| 3:C:1381:LEU:HD11 | 3:C:1383:ILE:CD1 | 2.32 | 0.54 |
| 3:C:1390:ALA:CB | 3:C:1416:PHE:HA | 2.37 | 0.54 |
| 3:C:1566:ILE:HG13 | 3:C:1569:ARG:HD3 | 1.90 | 0.54 |
| 3:C:1414:LYS:O | 3:C:1415:ALA:HB3 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:1337:ASN:HB2 | 3:F:1338:LYS:HD2 | 1.89 | 0.54 |
| 3:F:1503:ASP:C | 3:F:1504:LYS:HD3 | 2.28 | 0.54 |
| 3:F:1512:ASP:O | 3:F:1513:LYS:C | 2.47 | 0.54 |
| 1:A:20:MET:HE1 | 1:A:35:VAL:CG1 | 2.38 | 0.53 |
| 3:C:1512:ASP:O | 3:C:1513:LYS:C | 2.47 | 0.53 |
| 1:D:453:PHE:HB2 | 1:D:493:VAL:CG2 | 2.38 | 0.53 |
| 2:E:756:LEU:C | 2:E:758:GLU:OE1 | 2.47 | 0.53 |
| 1:A:392:HIS:CB | 1:A:393:PRO:CD | 2.59 | 0.53 |
| 2:B:819:ARG:HG2 | 2:B:819:ARG:NH1 | 2.14 | 0.53 |
| 2:B:838:LEU:HD22 | 2:B:894:VAL:HG21 | 1.90 | 0.53 |
| 1:A:3:MET:CE | 1:A:522:ARG:HG2 | 2.31 | 0.53 |
| 1:A:558:GLN:HB3 | 2:B:772:PHE:CE1 | 2.43 | 0.53 |
| 1:D:312:SER:HB2 | 1:D:314:SER:OG | 2.08 | 0.53 |
| 2:E:834:GLN:HE21 | 2:E:834:GLN:HA | 1.73 | 0.53 |
| 3:F:1462:ASN:ND2 | 3:F:1465:GLU:H | 2.06 | 0.53 |
| 4:H:61:ASP:OD2 | 4:H:64:SER:OG | 2.27 | 0.53 |
| 3:C:1503:ASP:C | 3:C:1504:LYS:HD3 | 2.28 | 0.53 |
| 3:F:1480:LEU:O | 3:F:1481:ASN:CB | 2.57 | 0.53 |
| 4:H:65:MET:O | 4:H:66:ALA:C | 2.46 | 0.53 |
| 2:E:767:LYS:HG2 | 2:E:768:LEU:N | 2.23 | 0.53 |
| 1:A:453:PHE:HB2 | 1:A:493:VAL:CG2 | 2.39 | 0.53 |
| 3:C:1381:LEU:HD21 | 3:C:1424:ILE:HB | 1.91 | 0.53 |
| 3:C:1411:GLU:OE2 | 3:C:1422:LEU:HA | 2.09 | 0.53 |
| 3:F:1341:LEU:HD12 | 3:F:1342:LYS:N | 2.24 | 0.53 |
| 3:F:1494:GLU:HG2 | 3:F:1602:LYS:CE | 2.39 | 0.53 |
| 1:D:578:LYS:HE3 | 2:E:800:GLU:OE2 | 2.09 | 0.53 |
| 1:A:290:GLN:HG2 | 3:F:1594:PRO:HG2 | 1.91 | 0.53 |
| 1:D:286:LEU:HD11 | 1:D:294:ALA:HB2 | 1.91 | 0.53 |
| 3:C:1393:THR:HG23 | 3:C:1419:ARG:HH22 | 1.74 | 0.52 |
| 3:F:1385:MET:HA | 3:F:1385:MET:CE | 2.39 | 0.52 |
| 3:C:1554:VAL:HB | 3:C:1560:ARG:CZ | 2.39 | 0.52 |
| 3:F:1380:ILE:HG13 | 3:F:1425:TYR:HD2 | 1.74 | 0.52 |
| 1:A:250:ILE:HB | 1:A:266:LEU:HD13 | 1.91 | 0.52 |
| 1:A:289:VAL:HG23 | 1:A:290:GLN:H | 1.74 | 0.52 |
| 3:C:1552:ASP:CG | 3:C:1554:VAL:CG1 | 2.75 | 0.52 |
| 1:D:250:ILE:HB | 1:D:266:LEU:HD13 | 1.91 | 0.52 |
| 3:F:1392:ASP:O | 3:F:1393:THR:C | 2.47 | 0.52 |
| 3:F:1407:ILE:HD11 | 3:F:1424:ILE:CD1 | 2.39 | 0.52 |
| 3:F:1497:PHE:HB3 | 3:F:1600:ILE:HG22 | 1.92 | 0.52 |
| 2:B:734:ILE:HG12 | 4:G:51:TYR:CD1 | 2.44 | 0.52 |
| 1:D:6:ILE:CG1 | 1:D:20:MET:HE3 | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:1364:LEU:HD11 | 3:F:1471:TYR:CE2 | 2.45 | 0.52 |
| 3:F:1383:ILE:HB | 3:F:1422:LEU:HD23 | 1.90 | 0.52 |
| 1:A:80:ARG:O | 1:A:81:ASN:HB2 | 2.10 | 0.52 |
| 1:A:164:LEU:O | 1:A:164:LEU:HD12 | 2.10 | 0.52 |
| 1:A:575:ALA:O | 2:B:748:SER:HA | 2.10 | 0.52 |
| 1:D:253:ILE:HD11 | 1:D:302:LEU:HD21 | 1.88 | 0.52 |
| 2:B:855:THR:HG23 | 2:B:858:ARG:HH12 | 1.74 | 0.52 |
| 3:C:1389:PHE:CD1 | 3:C:1443:GLN:CB | 2.92 | 0.52 |
| 1:A:517:GLY:O | 1:A:518:ALA:C | 2.46 | 0.52 |
| 1:D:282:ARG:HG2 | 1:D:282:ARG:HH11 | 1.75 | 0.52 |
| 1:D:372:GLU:HA | 1:D:373:ASP:HB3 | 1.88 | 0.52 |
| 2:E:836:GLN:NE2 | 2:E:897:HIS:CE1 | 2.71 | 0.52 |
| 3:F:1481:ASN:O | 3:F:1492:ALA:HB3 | 2.10 | 0.52 |
| 3:F:1521:TYR:OH | 3:F:1584:GLY:HA3 | 2.10 | 0.52 |
| 3:F:1618:GLU:C | 3:F:1621:GLN:HG3 | 2.30 | 0.52 |
| 1:A:372:GLU:HA | 1:A:373:ASP:HB3 | 1.88 | 0.52 |
| 4:H:61:ASP:CB | 4:H:64:SER:OG | 2.58 | 0.52 |
| 1:A:220:PHE:CD2 | 1:A:357:PRO:HG2 | 2.45 | 0.52 |
| 1:D:20:MET:HE1 | 1:D:35:VAL:CG1 | 2.39 | 0.52 |
| 2:E:734:ILE:HG12 | 4:H:51:TYR:HD1 | 1.70 | 0.52 |
| 2:E:860:HIS:HE1 | 3:F:1451:GLN:NE2 | 2.07 | 0.52 |
| 3:C:1389:PHE:CE1 | 3:C:1443:GLN:CB | 2.85 | 0.51 |
| 3:C:1521:TYR:OH | 3:C:1584:GLY:HA3 | 2.10 | 0.51 |
| 1:D:220:PHE:CD2 | 1:D:357:PRO:HG2 | 2.45 | 0.51 |
| 1:D:551:ARG:HE | 1:D:551:ARG:H | 1.56 | 0.51 |
| 1:D:590:THR:HG22 | 1:D:592:SER:N | 2.25 | 0.51 |
| 3:F:1558:GLN:O | 3:F:1559:GLN:HB3 | 2.10 | 0.51 |
| 3:C:1386:MET:HB3 | 3:C:1450:ILE:CG2 | 2.41 | 0.51 |
| 3:C:1490:ARG:HG3 | 3:C:1491:CYS:N | 2.25 | 0.51 |
| 3:C:1544:GLU:O | 3:C:1556:VAL:HG11 | 2.10 | 0.51 |
| 3:C:1614:GLU:C | 3:C:1616:GLN:H | 2.14 | 0.51 |
| 1:D:591:GLN:O | 1:D:594:ILE:HB | 2.10 | 0.51 |
| 2:E:894:VAL:HG22 | 2:E:897:HIS:HB2 | 1.92 | 0.51 |
| 1:A:6:ILE:CG1 | 1:A:20:MET:HE3 | 2.40 | 0.51 |
| 1:A:289:VAL:HG21 | 1:A:297:LEU:HD21 | 1.91 | 0.51 |
| 1:A:472:ILE:CD1 | 1:A:509:LEU:HD22 | 2.41 | 0.51 |
| 1:D:164:LEU:HD12 | 1:D:164:LEU:O | 2.10 | 0.51 |
| 3:F:1437:LEU:O | 3:F:1437:LEU:HG | 2.09 | 0.51 |
| 3:F:1563:ILE:HG13 | 3:F:1599:ILE:HD13 | 1.92 | 0.51 |
| 1:A:282:ARG:HG2 | 1:A:282:ARG:HH11 | 1.75 | 0.51 |
| 3:C:1558:GLN:O | 3:C:1559:GLN:HB3 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:1363:ILE:HG12 | 3:C:1440:LYS:HG3 | 1.93 | 0.51 |
| 3:C:1460:TYR:CZ | 3:C:1461:TYR:HB3 | 2.46 | 0.51 |
| 1:A:590:THR:HG22 | 1:A:592:SER:N | 2.26 | 0.51 |
| 3:F:1380:ILE:HB | 3:F:1458:TYR:CE1 | 2.46 | 0.51 |
| 3:F:1552:ASP:C | 3:F:1552:ASP:OD1 | 2.49 | 0.51 |
| 1:A:177:VAL:HG22 | 1:A:178:ASN:N | 2.26 | 0.51 |
| 3:C:1563:ILE:HG13 | 3:C:1599:ILE:HD13 | 1.92 | 0.51 |
| 1:D:177:VAL:HG22 | 1:D:178:ASN:N | 2.26 | 0.51 |
| 3:F:1443:GLN:O | 3:F:1443:GLN:HG2 | 2.11 | 0.51 |
| 1:A:474:ASN:HB3 | 1:A:477:ARG:NH1 | 2.26 | 0.51 |
| 3:C:1339:PHE:CE1 | 3:C:1370:TYR:CE1 | 2.99 | 0.51 |
| 1:D:345:GLY:N | 1:D:391:THR:HB | 2.26 | 0.51 |
| 1:D:474:ASN:OD1 | 1:D:475:LYS:HG3 | 2.10 | 0.51 |
| 3:F:1343:VAL:HG11 | 3:F:1471:TYR:HD2 | 1.76 | 0.51 |
| 1:A:69:PRO:CA | 1:A:70:ALA:CB | 2.88 | 0.51 |
| 1:A:346:MET:O | 1:A:347:PRO:C | 2.49 | 0.51 |
| 1:A:364:ARG:H | 1:A:379:THR:HG22 | 1.75 | 0.51 |
| 3:C:1593:LYS:N | 3:C:1596:LEU:HD21 | 2.26 | 0.51 |
| 1:D:69:PRO:CA | 1:D:70:ALA:CB | 2.88 | 0.51 |
| 1:D:158:LEU:CD2 | 1:D:167:LEU:HD22 | 2.41 | 0.51 |
| 3:F:1472:HIS:ND1 | 3:F:1473:PRO:CD | 2.73 | 0.51 |
| 3:F:1601:GLY:H | 3:F:1604:THR:HB | 1.76 | 0.51 |
| 3:C:1463:LEU:O | 3:C:1463:LEU:HG | 2.11 | 0.50 |
| 3:C:1537:ASP:CG | 3:C:1569:ARG:HD2 | 2.32 | 0.50 |
| 1:D:472:ILE:CD1 | 1:D:509:LEU:HD22 | 2.41 | 0.50 |
| 2:B:730:ASP:HB2 | 2:B:841:ARG:HH21 | 1.77 | 0.50 |
| 3:C:1380:ILE:HG13 | 3:C:1425:TYR:HD1 | 1.75 | 0.50 |
| 3:C:1406:TYR:OH | 3:C:1408:SER:HA | 2.11 | 0.50 |
| 1:D:126:ARG:HG3 | 2:E:751:TRP:CZ2 | 2.46 | 0.50 |
| 3:F:1462:ASN:ND2 | 3:F:1465:GLU:HG2 | 2.26 | 0.50 |
| 3:F:1582:MET:HB3 | 3:F:1605:TRP:O | 2.11 | 0.50 |
| 3:C:1476:GLU:O | 3:C:1477:ASP:C | 2.48 | 0.50 |
| 1:D:37:VAL:O | 1:D:46:VAL:HG23 | 2.11 | 0.50 |
| 1:D:223:ILE:HD12 | 1:D:223:ILE:N | 2.26 | 0.50 |
| 1:A:591:GLN:O | 1:A:594:ILE:HB | 2.10 | 0.50 |
| 3:F:1537:ASP:CG | 3:F:1569:ARG:HD2 | 2.31 | 0.50 |
| 1:A:158:LEU:CD2 | 1:A:167:LEU:HD22 | 2.41 | 0.50 |
| 1:A:474:ASN:OD1 | 1:A:475:LYS:HG3 | 2.11 | 0.50 |
| 1:A:564:GLU:HG2 | 2:B:766:THR:HG23 | 1.94 | 0.50 |
| 3:F:1483:LEU:O | 3:F:1484:CYS:SG | 2.69 | 0.50 |
| 3:F:1498:ILE:O | 3:F:1499:GLN:C | 2.49 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:223:ILE:HD12 | 1:A:223:ILE:N | 2.26 | 0.50 |
| 3:C:1493:GLU:OE1 | 3:C:1493:GLU:O | 2.30 | 0.50 |
| 3:F:1459:ALA:O | 3:F:1460:TYR:C | 2.50 | 0.50 |
| 3:F:1524:LYS:HB3 | 3:F:1545:GLN:HG2 | 1.94 | 0.50 |
| 1:A:445:PRO:HG2 | 1:A:504:ILE:HD11 | 1.94 | 0.50 |
| 2:B:758:GLU:OE2 | 2:B:767:LYS:HE2 | 2.12 | 0.50 |
| 3:C:1582:MET:HB3 | 3:C:1605:TRP:O | 2.11 | 0.50 |
| 3:C:1499:GLN:O | 3:C:1499:GLN:OE1 | 2.30 | 0.50 |
| 1:D:80:ARG:O | 1:D:81:ASN:HB2 | 2.10 | 0.50 |
| 3:F:1401:ASN:O | 3:F:1402:GLY:O | 2.29 | 0.50 |
| 3:F:1404:ASP:CB | 3:F:1427:ASP:HB2 | 2.41 | 0.50 |
| 3:F:1414:LYS:O | 3:F:1415:ALA:CB | 2.59 | 0.50 |
| 3:C:1397:LYS:N | 3:C:1397:LYS:CD | 2.75 | 0.49 |
| 3:C:1413:ASP:OD1 | 3:C:1413:ASP:O | 2.30 | 0.49 |
| 1:D:445:PRO:HG2 | 1:D:504:ILE:HD11 | 1.94 | 0.49 |
| 1:D:474:ASN:HB3 | 1:D:477:ARG:NH1 | 2.26 | 0.49 |
| 3:F:1572:LEU:HD22 | 3:F:1574:LEU:CD2 | 2.42 | 0.49 |
| 3:F:1616:GLN:OE1 | 3:F:1616:GLN:CA | 2.61 | 0.49 |
| 1:A:543:VAL:HG12 | 2:B:799:PHE:CD2 | 2.47 | 0.49 |
| 2:B:733:ILE:HG12 | 2:B:734:ILE:H | 1.77 | 0.49 |
| 3:C:1380:ILE:CG2 | 3:C:1381:LEU:N | 2.74 | 0.49 |
| 1:D:364:ARG:H | 1:D:379:THR:HG22 | 1.75 | 0.49 |
| 3:C:1640:PRO:O | 3:C:1641:ASN:O | 2.30 | 0.49 |
| 3:F:1482:LYS:NZ | 3:F:1484:CYS:SG | 2.85 | 0.49 |
| 3:F:1555:GLN:O | 3:F:1556:VAL:C | 2.50 | 0.49 |
| 1:A:37:VAL:O | 1:A:46:VAL:HG23 | 2.11 | 0.49 |
| 3:C:1370:TYR:O | 3:C:1431:HIS:HB2 | 2.13 | 0.49 |
| 3:C:1505:VAL:HG23 | 3:C:1505:VAL:O | 2.13 | 0.49 |
| 3:C:1601:GLY:H | 3:C:1604:THR:HB | 1.76 | 0.49 |
| 1:D:548:SER:O | 1:D:549:GLU:O | 2.30 | 0.49 |
| 3:F:1344:THR:HG23 | 3:F:1346:LYS:HE2 | 1.92 | 0.49 |
| 3:F:1407:ILE:CG1 | 3:F:1424:ILE:HG12 | 2.42 | 0.49 |
| 1:A:110:ILE:HG12 | 1:A:127:ILE:HG12 | 1.93 | 0.49 |
| 1:A:379:THR:HA | 1:A:385:ALA:HB2 | 1.94 | 0.49 |
| 3:C:1365:GLU:C | 3:C:1366:ILE:HG13 | 2.33 | 0.49 |
| 3:C:1632:GLU:O | 3:C:1636:VAL:HG23 | 2.13 | 0.49 |
| 1:D:3:MET:CE | 1:D:522:ARG:HG2 | 2.31 | 0.49 |
| 1:D:110:ILE:HG12 | 1:D:127:ILE:HG12 | 1.94 | 0.49 |
| 3:C:1393:THR:O | 3:C:1396:LEU:HB2 | 2.13 | 0.49 |
| 3:C:1554:VAL:HB | 3:C:1560:ARG:NH1 | 2.28 | 0.49 |
| 3:F:1381:LEU:HB2 | 3:F:1424:ILE:O | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:1543:ILE:CD1 | 3:F:1554:VAL:HG21 | 2.29 | 0.49 |
| 3:C:1390:ALA:HB1 | 3:C:1416:PHE:HA | 1.94 | 0.49 |
| 3:C:1521:TYR:O | 3:C:1583:TRP:HB2 | 2.13 | 0.49 |
| 3:C:1524:LYS:HB3 | 3:C:1545:GLN:HG2 | 1.94 | 0.49 |
| 3:C:1544:GLU:C | 3:C:1556:VAL:HG13 | 2.33 | 0.49 |
| 3:F:1386:MET:SD | 3:F:1473:PRO:HD3 | 2.53 | 0.49 |
| 1:A:142:MET:CG | 1:A:187:TYR:CE1 | 2.96 | 0.49 |
| 3:C:1507:LEU:C | 3:C:1507:LEU:HD13 | 2.33 | 0.49 |
| 1:D:282:ARG:NH1 | 1:D:286:LEU:HD12 | 2.27 | 0.49 |
| 1:D:379:THR:HA | 1:D:385:ALA:HB2 | 1.94 | 0.49 |
| 3:F:1507:LEU:HD13 | 3:F:1507:LEU:C | 2.33 | 0.49 |
| 1:D:142:MET:CG | 1:D:187:TYR:CE1 | 2.96 | 0.49 |
| 3:C:1381:LEU:HD12 | 3:C:1381:LEU:C | 2.32 | 0.48 |
| 3:C:1545:GLN:HA | 3:C:1556:VAL:CG1 | 2.42 | 0.48 |
| 3:C:1572:LEU:HD22 | 3:C:1574:LEU:CD2 | 2.42 | 0.48 |
| 1:D:188:TYR:HB2 | 1:D:191:SER:OG | 2.12 | 0.48 |
| 2:E:847:ASN:ND2 | 2:E:849:ALA:HB3 | 2.28 | 0.48 |
| 1:A:188:TYR:HB2 | 1:A:191:SER:OG | 2.12 | 0.48 |
| 1:A:291:ASN:OD1 | 3:F:1594:PRO:HD3 | 2.13 | 0.48 |
| 3:C:1462:ASN:C | 3:C:1462:ASN:HD22 | 2.17 | 0.48 |
| 1:D:346:MET:H | 1:D:391:THR:HB | 1.78 | 0.48 |
| 1:D:396:LYS:HG2 | 1:D:397:PRO:O | 2.14 | 0.48 |
| 2:E:730:ASP:HB2 | 2:E:841:ARG:NH2 | 2.27 | 0.48 |
| 3:F:1365:GLU:CG | 3:F:1438:ALA:HB2 | 2.43 | 0.48 |
| 3:F:1521:TYR:O | 3:F:1583:TRP:HB2 | 2.13 | 0.48 |
| 1:D:559:MET:HG3 | 1:D:560:THR:N | 2.28 | 0.48 |
| 3:F:1632:GLU:O | 3:F:1636:VAL:HG23 | 2.12 | 0.48 |
| 1:A:282:ARG:NH1 | 1:A:286:LEU:HD12 | 2.27 | 0.48 |
| 3:C:1537:ASP:OD2 | 3:C:1569:ARG:CD | 2.61 | 0.48 |
| 3:F:1483:LEU:HD12 | 3:F:1483:LEU:C | 2.33 | 0.48 |
| 3:F:1505:VAL:O | 3:F:1505:VAL:HG23 | 2.13 | 0.48 |
| 3:C:1370:TYR:N | 3:C:1430:SER:O | 2.35 | 0.48 |
| 1:D:236:ARG:CA | 1:D:243:VAL:HG23 | 2.44 | 0.48 |
| 3:F:1481:ASN:ND2 | 3:F:1567:LYS:HE3 | 2.29 | 0.48 |
| 1:A:109:PHE:CZ | 1:A:594:ILE:HG23 | 2.49 | 0.48 |
| 2:B:894:VAL:HG22 | 2:B:897:HIS:HB2 | 1.95 | 0.48 |
| 3:C:1467:CYS:SG | 3:C:1468:THR:N | 2.87 | 0.48 |
| 2:E:730:ASP:HB2 | 2:E:841:ARG:HH21 | 1.76 | 0.48 |
| 3:F:1537:ASP:OD2 | 3:F:1569:ARG:CD | 2.61 | 0.48 |
| 3:F:1572:LEU:O | 3:F:1573:LYS:HG3 | 2.14 | 0.48 |
| 1:A:559:MET:HG3 | 1:A:560:THR:N | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:33:VAL:HA | 1:D:89:THR:O | 2.14 | 0.48 |
| 2:E:819:ARG:CG | 2:E:819:ARG:NH1 | 2.71 | 0.48 |
| 2:E:898:PHE:O | 4:H:48:MET:HG3 | 2.14 | 0.48 |
| 3:F:1364:LEU:HD21 | 3:F:1471:TYR:CE2 | 2.49 | 0.48 |
| 3:C:1380:ILE:CG1 | 3:C:1425:TYR:CD1 | 2.96 | 0.48 |
| 3:C:1437:LEU:HD12 | 3:C:1438:ALA:N | 2.29 | 0.48 |
| 1:D:109:PHE:CZ | 1:D:594:ILE:HG23 | 2.49 | 0.48 |
| 3:F:1348:ALA:HB1 | 3:F:1349:PRO:HD2 | 1.96 | 0.48 |
| 1:A:24:ALA:HB3 | 1:A:60:HIS:CB | 2.38 | 0.47 |
| 1:D:369:VAL:HG12 | 1:D:370:GLN:H | 1.79 | 0.47 |
| 2:E:761:LYS:O | 2:E:762:ASN:CG | 2.53 | 0.47 |
| 3:F:1371:ARG:NH1 | 3:F:1371:ARG:CG | 2.75 | 0.47 |
| 3:F:1462:ASN:HD22 | 3:F:1464:GLU:N | 2.10 | 0.47 |
| 1:A:171:TRP:CZ3 | 1:A:173:ILE:HG12 | 2.49 | 0.47 |
| 1:A:177:VAL:HG22 | 1:A:182:TRP:HZ2 | 1.78 | 0.47 |
| 3:C:1411:GLU:O | 3:C:1413:ASP:N | 2.47 | 0.47 |
| 3:C:1494:GLU:H | 3:C:1494:GLU:HG2 | 1.47 | 0.47 |
| 1:D:438:VAL:HG21 | 1:D:449:LEU:HD21 | 1.96 | 0.47 |
| 2:E:731:GLU:O | 2:E:732:ASP:CB | 2.62 | 0.47 |
| 1:A:365:VAL:H | 1:A:379:THR:HG22 | 1.79 | 0.47 |
| 2:B:772:PHE:CZ | 4:G:82:ILE:HD13 | 2.50 | 0.47 |
| 2:B:862:GLN:N | 2:B:862:GLN:OE1 | 2.47 | 0.47 |
| 3:C:1341:LEU:HD22 | 3:C:1457:VAL:HG22 | 1.97 | 0.47 |
| 3:C:1572:LEU:O | 3:C:1573:LYS:HG3 | 2.14 | 0.47 |
| 1:D:177:VAL:HG22 | 1:D:182:TRP:HZ2 | 1.78 | 0.47 |
| 1:D:333:ILE:HD11 | 1:D:404:THR:HG22 | 1.97 | 0.47 |
| 2:B:731:GLU:O | 2:B:732:ASP:HB2 | 2.13 | 0.47 |
| 3:C:1616:GLN:O | 3:C:1617:ASP:C | 2.53 | 0.47 |
| 1:D:171:TRP:CZ3 | 1:D:173:ILE:HG12 | 2.49 | 0.47 |
| 1:D:335:PHE:CE1 | 1:D:419:MET:HG2 | 2.50 | 0.47 |
| 3:F:1513:LYS:O | 3:F:1515:CYS:N | 2.48 | 0.47 |
| 1:A:369:VAL:HG12 | 1:A:370:GLN:H | 1.79 | 0.47 |
| 1:A:398:LEU:O | 1:A:420:GLN:HA | 2.15 | 0.47 |
| 2:B:730:ASP:HB2 | 2:B:841:ARG:NH2 | 2.29 | 0.47 |
| 1:D:36:THR:HG22 | 1:D:38:HIS:CE1 | 2.50 | 0.47 |
| 1:A:33:VAL:HA | 1:A:89:THR:O | 2.14 | 0.47 |
| 1:A:158:LEU:HD12 | 1:A:159:SER:H | 1.80 | 0.47 |
| 3:C:1397:LYS:HA | 3:C:1400:ALA:CB | 2.43 | 0.47 |
| 3:C:1572:LEU:C | 3:C:1573:LYS:HG3 | 2.35 | 0.47 |
| 1:D:292:PRO:HB2 | 1:D:296:ASP:OD2 | 2.13 | 0.47 |
| 3:F:1341:LEU:HD22 | 3:F:1457:VAL:CG2 | 2.42 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:1581:LEU:HD12 | 3:F:1582:MET:H | 1.80 | 0.47 |
| 1:A:3:MET:HE3 | 1:A:522:ARG:CG | 2.32 | 0.47 |
| 1:A:335:PHE:CE1 | 1:A:419:MET:HG2 | 2.50 | 0.47 |
| 3:C:1378:MET:CA | 3:C:1427:ASP:O | 2.52 | 0.47 |
| 1:D:158:LEU:HD12 | 1:D:159:SER:H | 1.80 | 0.47 |
| 1:D:204:GLU:CG | 2:E:815:TYR:CE2 | 2.98 | 0.47 |
| 1:D:398:LEU:O | 1:D:420:GLN:HA | 2.15 | 0.47 |
| 2:E:862:GLN:N | 2:E:862:GLN:OE1 | 2.47 | 0.47 |
| 3:F:1498:ILE:CG2 | 3:F:1499:GLN:N | 2.78 | 0.47 |
| 3:F:1512:ASP:O | 3:F:1515:CYS:N | 2.47 | 0.47 |
| 3:F:1572:LEU:C | 3:F:1573:LYS:HG3 | 2.35 | 0.47 |
| 1:A:338:THR:HG21 | 1:A:419:MET:CE | 2.45 | 0.47 |
| 3:C:1472:HIS:CG | 3:C:1475:LYS:HD2 | 2.48 | 0.47 |
| 3:F:1462:ASN:CG | 3:F:1465:GLU:HG2 | 2.34 | 0.47 |
| 1:A:363:TYR:O | 1:A:364:ARG:HB2 | 2.14 | 0.47 |
| 1:A:548:SER:O | 1:A:549:GLU:CB | 2.62 | 0.47 |
| 3:C:1527:LEU:HD11 | 3:C:1539:TYR:HB3 | 1.96 | 0.47 |
| 1:D:61:MET:HE1 | 1:D:482:GLY:C | 2.34 | 0.47 |
| 1:D:151:ILE:N | 1:D:151:ILE:HD12 | 2.30 | 0.47 |
| 1:D:344:PRO:HA | 1:D:391:THR:CG2 | 2.45 | 0.47 |
| 1:D:427:VAL:HG21 | 1:D:523:GLU:HG3 | 1.97 | 0.47 |
| 3:F:1345:ILE:HA | 3:F:1363:ILE:O | 2.15 | 0.47 |
| 3:F:1360:ASN:C | 3:F:1361:THR:HG23 | 2.35 | 0.47 |
| 3:F:1380:ILE:HD13 | 3:F:1458:TYR:HE1 | 1.79 | 0.47 |
| 3:F:1618:GLU:HA | 3:F:1621:GLN:CD | 2.33 | 0.47 |
| 1:A:404:THR:HG21 | 1:A:415:ALA:H | 1.81 | 0.47 |
| 1:A:438:VAL:HG21 | 1:A:449:LEU:HD21 | 1.95 | 0.47 |
| 3:C:1497:PHE:HE2 | 3:C:1571:ALA:CB | 2.25 | 0.47 |
| 3:F:1527:LEU:HD11 | 3:F:1539:TYR:HB3 | 1.96 | 0.47 |
| 1:A:541:LEU:HD23 | 2:B:796:ALA:HB2 | 1.97 | 0.46 |
| 2:B:809:ILE:HD13 | 2:B:890:VAL:HG23 | 1.96 | 0.46 |
| 3:C:1380:ILE:CG1 | 3:C:1425:TYR:HD1 | 2.28 | 0.46 |
| 3:C:1481:ASN:ND2 | 3:C:1567:LYS:HE2 | 2.31 | 0.46 |
| 1:D:7:ILE:HG21 | 1:D:471:LEU:CD2 | 2.45 | 0.46 |
| 1:D:338:THR:HG21 | 1:D:419:MET:CE | 2.45 | 0.46 |
| 1:D:363:TYR:O | 1:D:364:ARG:HB2 | 2.14 | 0.46 |
| 3:F:1481:ASN:C | 3:F:1492:ALA:HB3 | 2.35 | 0.46 |
| 1:A:151:ILE:N | 1:A:151:ILE:HD12 | 2.30 | 0.46 |
| 1:A:558:GLN:CB | 2:B:772:PHE:CE1 | 2.98 | 0.46 |
| 1:D:365:VAL:H | 1:D:379:THR:HG22 | 1.79 | 0.46 |
| 2:E:851:CYS:HB2 | 2:E:881:LEU:HD21 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:7:ILE:HG21 | 1:A:471:LEU:CD2 | 2.45 | 0.46 |
| 3:C:1541:MET:O | 3:C:1559:GLN:HA | 2.16 | 0.46 |
| 1:D:404:THR:HG21 | 1:D:415:ALA:H | 1.80 | 0.46 |
| 1:D:549:GLU:CG | 1:D:550:ASP:H | 2.28 | 0.46 |
| 1:A:292:PRO:HG2 | 1:A:296:ASP:OD2 | 2.15 | 0.46 |
| 1:A:134:LEU:HD13 | 2:B:793:ILE:HG22 | 1.96 | 0.46 |
| 1:A:236:ARG:CA | 1:A:243:VAL:HG23 | 2.44 | 0.46 |
| 1:A:543:VAL:O | 2:B:799:PHE:CG | 2.68 | 0.46 |
| 2:B:758:GLU:OE2 | 2:B:767:LYS:CE | 2.63 | 0.46 |
| 3:C:1385:MET:HE3 | 3:C:1385:MET:HA | 1.97 | 0.46 |
| 1:D:54:LEU:HB3 | 1:D:60:HIS:HA | 1.98 | 0.46 |
| 3:F:1404:ASP:O | 3:F:1405:ARG:HG2 | 2.16 | 0.46 |
| 1:A:214:VAL:HB | 1:A:233:ILE:HD13 | 1.98 | 0.46 |
| 1:A:250:ILE:HG13 | 1:A:266:LEU:HB2 | 1.97 | 0.46 |
| 3:C:1396:LEU:CB | 3:C:1412:LEU:HD12 | 2.36 | 0.46 |
| 3:C:1397:LYS:H | 3:C:1397:LYS:CD | 2.28 | 0.46 |
| 3:C:1411:GLU:C | 3:C:1413:ASP:N | 2.69 | 0.46 |
| 1:A:469:THR:O | 1:A:511:ALA:HA | 2.16 | 0.46 |
| 3:F:1641:ASN:N | 3:F:1641:ASN:HD22 | 2.13 | 0.46 |
| 1:A:135:LEU:HD22 | 2:B:789:ASP:O | 2.16 | 0.46 |
| 2:B:739:ILE:CG2 | 2:B:891:LYS:HD3 | 2.46 | 0.46 |
| 1:D:255:ASP:HA | 1:D:256:GLY:HA2 | 1.63 | 0.46 |
| 3:F:1447:VAL:HG22 | 3:F:1448:GLU:N | 2.31 | 0.46 |
| 3:F:1541:MET:O | 3:F:1559:GLN:HA | 2.16 | 0.46 |
| 2:B:739:ILE:HD11 | 2:B:900:SER:HB2 | 1.97 | 0.46 |
| 3:C:1416:PHE:CZ | 3:C:1442:HIS:HB2 | 2.51 | 0.46 |
| 3:C:1485:ARG:CD | 3:C:1536:PHE:CE2 | 2.99 | 0.46 |
| 1:D:214:VAL:HB | 1:D:233:ILE:HD13 | 1.98 | 0.46 |
| 1:D:469:THR:O | 1:D:511:ALA:HA | 2.16 | 0.46 |
| 2:B:762:ASN:C | 2:B:764:ILE:H | 2.20 | 0.46 |
| 1:D:572:VAL:HG12 | 2:E:753:VAL:HG22 | 1.96 | 0.46 |
| 3:F:1386:MET:O | 3:F:1387:THR:C | 2.55 | 0.46 |
| 3:F:1413:ASP:O | 3:F:1413:ASP:OD2 | 2.34 | 0.46 |
| 1:A:177:VAL:CG2 | 1:A:182:TRP:HZ2 | 2.30 | 0.45 |
| 1:A:477:ARG:HH11 | 1:A:477:ARG:CG | 2.30 | 0.45 |
| 1:A:541:LEU:HB3 | 2:B:796:ALA:HB2 | 1.98 | 0.45 |
| 3:C:1494:GLU:HB2 | 3:C:1495:ASN:H | 1.53 | 0.45 |
| 3:C:1590:TRP:O | 3:C:1596:LEU:HA | 2.16 | 0.45 |
| 1:D:250:ILE:HG13 | 1:D:266:LEU:HB2 | 1.97 | 0.45 |
| 3:F:1461:TYR:CD1 | 3:F:1462:ASN:HB2 | 2.51 | 0.45 |
| 1:A:61:MET:HE1 | 1:A:482:GLY:C | 2.36 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:292:PRO:CD | 1:A:296:ASP:OD2 | 2.64 | 0.45 |
| 1:A:333:ILE:HD11 | 1:A:404:THR:HG22 | 1.97 | 0.45 |
| 1:A:427:VAL:HG21 | 1:A:523:GLU:HG3 | 1.97 | 0.45 |
| 3:C:1343:VAL:CG2 | 3:C:1366:ILE:HG23 | 2.31 | 0.45 |
| 3:F:1452:PRO:HG3 | 3:F:1472:HIS:HD2 | 1.81 | 0.45 |
| 1:A:216:PRO:HB2 | 1:A:218:GLU:O | 2.16 | 0.45 |
| 1:A:338:THR:HG21 | 1:A:419:MET:HE1 | 1.98 | 0.45 |
| 2:B:761:LYS:O | 2:B:762:ASN:CB | 2.64 | 0.45 |
| 1:D:24:ALA:HB3 | 1:D:60:HIS:CB | 2.38 | 0.45 |
| 1:D:216:PRO:HB2 | 1:D:218:GLU:O | 2.16 | 0.45 |
| 1:D:286:LEU:HD23 | 1:D:286:LEU:HA | 1.60 | 0.45 |
| 1:D:443:LEU:HD23 | 1:D:443:LEU:HA | 1.81 | 0.45 |
| 1:D:549:GLU:CG | 1:D:550:ASP:N | 2.79 | 0.45 |
| 3:C:1495:ASN:ND2 | 3:C:1496:CYS:H | 2.10 | 0.45 |
| 1:D:289:VAL:HG23 | 1:D:290:GLN:N | 2.32 | 0.45 |
| 3:F:1386:MET:HG3 | 3:F:1471:TYR:HE1 | 1.81 | 0.45 |
| 3:F:1463:LEU:O | 3:F:1463:LEU:HD23 | 2.17 | 0.45 |
| 1:A:36:THR:HG22 | 1:A:38:HIS:CE1 | 2.50 | 0.45 |
| 1:A:54:LEU:HB3 | 1:A:60:HIS:HA | 1.98 | 0.45 |
| 1:A:59:ASN:O | 1:A:60:HIS:HB2 | 2.17 | 0.45 |
| 2:B:868:PRO:O | 2:B:869:LYS:C | 2.55 | 0.45 |
| 1:D:409:LEU:HB3 | 1:D:410:SER:H | 1.63 | 0.45 |
| 1:D:477:ARG:HH11 | 1:D:477:ARG:CG | 2.30 | 0.45 |
| 3:F:1460:TYR:CZ | 3:F:1461:TYR:HB3 | 2.51 | 0.45 |
| 1:D:56:PRO:HD3 | 1:D:60:HIS:HE1 | 1.82 | 0.45 |
| 1:D:136:PRO:HD2 | 2:E:789:ASP:HA | 1.99 | 0.45 |
| 1:D:503:PHE:HD1 | 1:D:507:PHE:CD1 | 2.35 | 0.45 |
| 3:F:1381:LEU:HD23 | 3:F:1457:VAL:HG12 | 1.92 | 0.45 |
| 3:F:1403:VAL:O | 3:F:1403:VAL:HG13 | 2.17 | 0.45 |
| 3:F:1482:LYS:HG2 | 3:F:1484:CYS:SG | 2.56 | 0.45 |
| 3:F:1528:VAL:HG23 | 3:F:1541:MET:HA | 1.98 | 0.45 |
| 1:A:126:ARG:HG3 | 2:B:751:TRP:CZ2 | 2.51 | 0.45 |
| 1:A:362:ALA:O | 1:A:379:THR:HG21 | 2.17 | 0.45 |
| 3:C:1462:ASN:HD22 | 3:C:1464:GLU:H | 1.65 | 0.45 |
| 3:C:1528:VAL:HG23 | 3:C:1541:MET:HA | 1.98 | 0.45 |
| 3:F:1374:GLN:O | 3:F:1375:ASP:O | 2.35 | 0.45 |
| 4:G:63:VAL:O | 4:G:67:ASP:HB2 | 2.16 | 0.45 |
| 1:A:567:HIS:ND1 | 2:B:760:PRO:HB3 | 2.32 | 0.45 |
| 1:D:177:VAL:CG2 | 1:D:182:TRP:HZ2 | 2.30 | 0.45 |
| 1:D:179:MET:HG3 | 1:D:203:LYS:HA | 1.99 | 0.45 |
| 3:F:1628:GLY:O | 3:F:1632:GLU:HG3 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:56:PRO:HD3 | 1:A:60:HIS:HE1 | 1.82 | 0.45 |
| 1:A:404:THR:HG23 | 1:A:415:ALA:H | 1.82 | 0.45 |
| 1:A:471:LEU:HD22 | 1:A:622:LEU:HD13 | 1.99 | 0.45 |
| 1:A:572:VAL:HG12 | 2:B:753:VAL:HG22 | 1.99 | 0.45 |
| 3:C:1453:GLY:HA3 | 3:C:1471:TYR:CE2 | 2.51 | 0.45 |
| 1:D:345:GLY:HA2 | 1:D:391:THR:O | 2.16 | 0.45 |
| 2:E:744:GLU:O | 2:E:746:PRO:HD2 | 2.17 | 0.45 |
| 3:F:1387:THR:CG2 | 3:F:1451:GLN:HB3 | 2.46 | 0.45 |
| 1:A:484:GLN:OE1 | 1:A:495:LEU:HB2 | 2.17 | 0.45 |
| 1:A:625:THR:HA | 1:A:631:GLN:HB3 | 1.99 | 0.45 |
| 1:D:59:ASN:O | 1:D:60:HIS:HB2 | 2.17 | 0.45 |
| 3:F:1497:PHE:CD1 | 3:F:1606:VAL:HB | 2.52 | 0.45 |
| 3:F:1593:LYS:CA | 3:F:1596:LEU:CD2 | 2.92 | 0.45 |
| 3:F:1614:GLU:O | 3:F:1620:ASN:CB | 2.64 | 0.45 |
| 2:B:847:ASN:ND2 | 2:B:849:ALA:HB3 | 2.31 | 0.44 |
| 3:C:1340:ASP:N | 3:C:1369:ARG:O | 2.50 | 0.44 |
| 1:D:293:ARG:O | 1:D:296:ASP:N | 2.45 | 0.44 |
| 2:E:855:THR:HG23 | 2:E:858:ARG:HH12 | 1.82 | 0.44 |
| 3:C:1408:SER:OG | 3:C:1410:TYR:HB3 | 2.16 | 0.44 |
| 3:C:1628:GLY:O | 3:C:1632:GLU:HG3 | 2.17 | 0.44 |
| 1:D:362:ALA:O | 1:D:379:THR:HG21 | 2.17 | 0.44 |
| 1:D:484:GLN:OE1 | 1:D:495:LEU:HB2 | 2.17 | 0.44 |
| 3:F:1382:ASP:HB3 | 3:F:1456:LYS:HB3 | 1.99 | 0.44 |
| 3:F:1408:SER:O | 3:F:1411:GLU:N | 2.48 | 0.44 |
| 3:F:1615:CYS:O | 3:F:1617:ASP:N | 2.50 | 0.44 |
| 1:A:6:ILE:HD11 | 1:A:20:MET:HG3 | 1.99 | 0.44 |
| 1:A:454:LEU:HD21 | 1:A:492:LEU:HD12 | 1.94 | 0.44 |
| 1:A:583:LEU:HD12 | 1:A:583:LEU:HA | 1.78 | 0.44 |
| 3:C:1404:ASP:HB3 | 3:C:1427:ASP:CB | 2.39 | 0.44 |
| 3:C:1617:ASP:O | 3:C:1621:GLN:HG3 | 2.18 | 0.44 |
| 2:E:895:TYR:C | 2:E:897:HIS:H | 2.19 | 0.44 |
| 1:A:286:LEU:HA | 1:A:286:LEU:HD23 | 1.60 | 0.44 |
| 1:A:503:PHE:HD1 | 1:A:507:PHE:CD1 | 2.35 | 0.44 |
| 2:B:758:GLU:O | 2:B:765:SER:OG | 2.35 | 0.44 |
| 2:B:894:VAL:HG11 | 2:B:899:ILE:HB | 1.99 | 0.44 |
| 1:D:6:ILE:HD11 | 1:D:20:MET:HG3 | 1.99 | 0.44 |
| 1:D:183:LYS:HZ2 | 1:D:185:ARG:CG | 2.31 | 0.44 |
| 1:D:471:LEU:HD22 | 1:D:622:LEU:HD13 | 1.99 | 0.44 |
| 2:B:750:LEU:C | 2:B:752:ASN:HD22 | 2.20 | 0.44 |
| 3:C:1621:GLN:O | 3:C:1625:GLN:HG3 | 2.17 | 0.44 |
| 1:D:329:SER:HA | 1:D:330:PRO:HD3 | 1.74 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:1483:LEU:O | 3:F:1489:CYS:SG | 2.76 | 0.44 |
| 3:C:1495:ASN:ND2 | 3:C:1496:CYS:N | 2.59 | 0.44 |
| 1:A:547:GLN:OE1 | 1:A:559:MET:CA | 2.65 | 0.44 |
| 1:D:193:GLN:H | 1:D:193:GLN:NE2 | 2.15 | 0.44 |
| 1:D:510:VAL:HB | 1:D:528:SER:HB3 | 2.00 | 0.44 |
| 1:A:179:MET:HG3 | 1:A:203:LYS:HA | 1.99 | 0.44 |
| 2:B:764:ILE:O | 2:B:764:ILE:HG22 | 2.18 | 0.44 |
| 2:B:772:PHE:HZ | 4:G:82:ILE:HD13 | 1.83 | 0.44 |
| 2:B:867:PRO:HB2 | 2:B:870:SER:OG | 2.17 | 0.44 |
| 2:B:895:TYR:C | 2:B:897:HIS:H | 2.19 | 0.44 |
| 1:D:375:VAL:HG12 | 1:D:376:GLN:H | 1.83 | 0.44 |
| 3:F:1617:ASP:O | 3:F:1621:GLN:HG2 | 2.18 | 0.44 |
| 1:A:223:ILE:HD12 | 1:A:223:ILE:H | 1.83 | 0.44 |
| 1:A:289:VAL:O | 1:A:290:GLN:HG2 | 2.17 | 0.44 |
| 1:A:454:LEU:HD21 | 1:A:492:LEU:CD1 | 2.48 | 0.44 |
| 2:B:910:VAL:CG2 | 2:B:911:PRO:HD2 | 2.45 | 0.44 |
| 3:C:1459:ALA:O | 3:C:1460:TYR:C | 2.56 | 0.44 |
| 1:D:179:MET:CE | 1:D:204:GLU:HG3 | 2.47 | 0.44 |
| 1:A:179:MET:CE | 1:A:204:GLU:HG3 | 2.47 | 0.43 |
| 3:C:1451:GLN:HA | 3:C:1452:PRO:HD3 | 1.78 | 0.43 |
| 3:C:1503:ASP:O | 3:C:1504:LYS:HB3 | 2.18 | 0.43 |
| 3:C:1615:CYS:C | 3:C:1616:GLN:OE1 | 2.57 | 0.43 |
| 1:D:47:LEU:O | 1:D:47:LEU:HD23 | 2.18 | 0.43 |
| 1:D:404:THR:HG23 | 1:D:415:ALA:H | 1.82 | 0.43 |
| 1:D:639:GLN:HE21 | 1:D:639:GLN:HB2 | 1.65 | 0.43 |
| 2:E:830:TYR:CD1 | 2:E:871:SER:HB3 | 2.53 | 0.43 |
| 3:F:1383:ILE:HB | 3:F:1422:LEU:CD2 | 2.48 | 0.43 |
| 3:F:1412:LEU:HA | 3:F:1412:LEU:HD12 | 1.61 | 0.43 |
| 3:F:1498:ILE:CG2 | 3:F:1499:GLN:HG2 | 2.48 | 0.43 |
| 3:F:1561:THR:O | 3:F:1598:TYR:N | 2.46 | 0.43 |
| 1:A:248:PHE:CD1 | 3:C:1378:MET:CE | 3.01 | 0.43 |
| 1:A:282:ARG:HG2 | 1:A:282:ARG:NH1 | 2.33 | 0.43 |
| 3:C:1593:LYS:HA | 3:C:1594:PRO:HA | 1.87 | 0.43 |
| 3:F:1483:LEU:HD12 | 3:F:1484:CYS:H | 1.76 | 0.43 |
| 1:A:6:ILE:HA | 1:A:6:ILE:HD12 | 1.68 | 0.43 |
| 1:A:47:LEU:HD23 | 1:A:47:LEU:O | 2.18 | 0.43 |
| 1:A:193:GLN:H | 1:A:193:GLN:NE2 | 2.15 | 0.43 |
| 1:A:290:GLN:OE1 | 3:F:1558:GLN:HG3 | 2.17 | 0.43 |
| 1:A:375:VAL:HG12 | 1:A:376:GLN:H | 1.83 | 0.43 |
| 2:B:731:GLU:O | 2:B:732:ASP:CB | 2.66 | 0.43 |
| 3:C:1360:ASN:C | 3:C:1361:THR:HG23 | 2.39 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:1552:ASP:OD1 | 3:C:1560:ARG:NH1 | 2.50 | 0.43 |
| 1:D:3:MET:HE3 | 1:D:522:ARG:CG | 2.33 | 0.43 |
| 2:E:733:ILE:HG12 | 2:E:734:ILE:H | 1.83 | 0.43 |
| 2:E:739:ILE:CG2 | 2:E:891:LYS:HD3 | 2.48 | 0.43 |
| 3:F:1380:ILE:HG13 | 3:F:1425:TYR:CD2 | 2.53 | 0.43 |
| 3:F:1405:ARG:HG2 | 3:F:1426:LEU:HD23 | 2.00 | 0.43 |
| 3:F:1414:LYS:O | 3:F:1415:ALA:HB3 | 2.19 | 0.43 |
| 3:F:1497:PHE:CD1 | 3:F:1606:VAL:HG21 | 2.53 | 0.43 |
| 3:F:1591:GLY:HA3 | 3:F:1596:LEU:HA | 2.00 | 0.43 |
| 1:A:124:LEU:HD23 | 1:A:124:LEU:HA | 1.77 | 0.43 |
| 3:C:1411:GLU:C | 3:C:1413:ASP:H | 2.22 | 0.43 |
| 3:C:1426:LEU:HD13 | 3:C:1426:LEU:H | 1.81 | 0.43 |
| 3:C:1446:ASN:N | 3:C:1446:ASN:HD22 | 2.16 | 0.43 |
| 1:D:505:PRO:O | 1:D:506:SER:HB3 | 2.17 | 0.43 |
| 3:F:1483:LEU:HD22 | 3:F:1599:ILE:HD11 | 2.00 | 0.43 |
| 1:A:409:LEU:HB3 | 1:A:410:SER:H | 1.63 | 0.43 |
| 2:B:739:ILE:CD1 | 2:B:900:SER:HB2 | 2.48 | 0.43 |
| 2:B:750:LEU:HD12 | 2:B:750:LEU:HA | 1.86 | 0.43 |
| 2:B:840:VAL:HG22 | 2:B:894:VAL:HB | 2.01 | 0.43 |
| 3:C:1366:ILE:HG22 | 3:C:1367:CYS:H | 1.84 | 0.43 |
| 3:C:1381:LEU:CD2 | 3:C:1383:ILE:HD11 | 2.49 | 0.43 |
| 4:G:41:TYR:HD2 | 4:G:42:TYR:CE2 | 2.37 | 0.43 |
| 1:A:63:ASN:C | 1:A:64:VAL:HG13 | 2.37 | 0.43 |
| 1:A:289:VAL:HG23 | 1:A:290:GLN:N | 2.33 | 0.43 |
| 1:A:363:TYR:HA | 1:A:379:THR:CG2 | 2.49 | 0.43 |
| 1:A:505:PRO:O | 1:A:506:SER:HB3 | 2.17 | 0.43 |
| 1:A:510:VAL:HB | 1:A:528:SER:HB3 | 2.00 | 0.43 |
| 3:C:1372:GLY:O | 3:C:1431:HIS:ND1 | 2.51 | 0.43 |
| 3:C:1462:ASN:ND2 | 3:C:1464:GLU:HB2 | 2.31 | 0.43 |
| 1:D:126:ARG:HG3 | 2:E:751:TRP:HZ2 | 1.82 | 0.43 |
| 1:D:282:ARG:HG2 | 1:D:282:ARG:NH1 | 2.33 | 0.43 |
| 1:A:329:SER:CB | 1:A:413:GLU:O | 2.61 | 0.43 |
| 2:B:760:PRO:O | 2:B:761:LYS:CG | 2.67 | 0.43 |
| 2:B:809:ILE:HD12 | 2:B:902:GLY:HA2 | 2.01 | 0.43 |
| 2:B:850:PHE:CD2 | 2:B:878:ILE:HD12 | 2.53 | 0.43 |
| 3:C:1389:PHE:CG | 3:C:1443:GLN:CA | 3.02 | 0.43 |
| 3:C:1443:GLN:O | 3:C:1443:GLN:OE1 | 2.37 | 0.43 |
| 3:C:1506:THR:OG1 | 3:C:1507:LEU:N | 2.52 | 0.43 |
| 1:D:363:TYR:HA | 1:D:379:THR:CG2 | 2.49 | 0.43 |
| 3:F:1397:LYS:HA | 3:F:1400:ALA:CB | 2.48 | 0.43 |
| 1:A:439:LEU:HD12 | 1:A:439:LEU:N | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:758:GLU:CD | 2:E:767:LYS:HB2 | 2.26 | 0.43 |
| 3:F:1474:GLU:O | 3:F:1475:LYS:C | 2.57 | 0.43 |
| 1:A:570:ARG:HA | 2:B:755:ASP:HA | 2.00 | 0.43 |
| 2:B:834:GLN:NE2 | 2:B:869:LYS:HD2 | 2.34 | 0.43 |
| 3:C:1440:LYS:HB2 | 3:C:1440:LYS:HE2 | 1.79 | 0.43 |
| 3:F:1408:SER:C | 3:F:1410:TYR:N | 2.72 | 0.43 |
| 4:H:41:TYR:HD2 | 4:H:42:TYR:CE2 | 2.37 | 0.43 |
| 1:A:343:LYS:HB2 | 1:A:346:MET:HB3 | 2.01 | 0.43 |
| 1:A:561:LEU:HD22 | 2:B:771:ILE:HD13 | 2.01 | 0.43 |
| 3:C:1396:LEU:HD13 | 3:C:1412:LEU:HD12 | 2.00 | 0.43 |
| 2:E:834:GLN:NE2 | 2:E:869:LYS:HD2 | 2.34 | 0.43 |
| 3:F:1386:MET:HE1 | 3:F:1389:PHE:CZ | 2.54 | 0.43 |
| 1:A:115:THR:HB | 1:A:584:ASN:OD1 | 2.19 | 0.42 |
| 2:B:744:GLU:O | 2:B:746:PRO:HD2 | 2.19 | 0.42 |
| 3:C:1576:GLU:O | 3:C:1577:LYS:HB2 | 2.18 | 0.42 |
| 2:E:841:ARG:HD3 | 2:E:861:GLN:HB2 | 2.00 | 0.42 |
| 3:F:1394:ASP:O | 3:F:1395:ASP:C | 2.57 | 0.42 |
| 1:A:47:LEU:HG | 1:A:48:SER:N | 2.34 | 0.42 |
| 1:A:375:VAL:HG12 | 1:A:376:GLN:N | 2.34 | 0.42 |
| 3:C:1381:LEU:HD22 | 3:C:1383:ILE:HD11 | 2.01 | 0.42 |
| 1:D:111:GLN:O | 1:D:125:TYR:HA | 2.19 | 0.42 |
| 1:D:291:ASN:N | 1:D:291:ASN:HD22 | 2.16 | 0.42 |
| 1:A:453:PHE:HB2 | 1:A:493:VAL:HG22 | 2.00 | 0.42 |
| 1:A:554:VAL:HG22 | 2:B:805:GLN:HG3 | 2.01 | 0.42 |
| 2:B:762:ASN:C | 2:B:764:ILE:N | 2.72 | 0.42 |
| 3:C:1403:VAL:HG13 | 3:C:1403:VAL:O | 2.20 | 0.42 |
| 3:C:1545:GLN:HA | 3:C:1556:VAL:HG11 | 2.00 | 0.42 |
| 1:D:183:LYS:HG2 | 1:D:199:GLU:HG2 | 2.01 | 0.42 |
| 1:D:459:ARG:HA | 1:D:462:GLU:HG2 | 2.01 | 0.42 |
| 3:F:1381:LEU:HD11 | 3:F:1437:LEU:HD21 | 2.00 | 0.42 |
| 3:F:1576:GLU:O | 3:F:1577:LYS:HB2 | 2.18 | 0.42 |
| 4:G:18:ALA:N | 4:G:65:MET:HE3 | 2.34 | 0.42 |
| 4:G:72:LEU:O | 4:G:73:GLU:C | 2.58 | 0.42 |
| 1:A:606:THR:C | 1:A:608:GLY:H | 2.22 | 0.42 |
| 2:B:855:THR:HB | 3:C:1602:LYS:NZ | 2.34 | 0.42 |
| 3:C:1408:SER:O | 3:C:1410:TYR:N | 2.53 | 0.42 |
| 3:C:1454:ALA:CB | 3:C:1470:PHE:CE2 | 2.95 | 0.42 |
| 1:D:40:PHE:HA | 1:D:41:PRO:HA | 1.76 | 0.42 |
| 1:D:115:THR:HB | 1:D:584:ASN:OD1 | 2.19 | 0.42 |
| 1:D:409:LEU:HD12 | 1:D:409:LEU:HA | 1.84 | 0.42 |
| 1:D:453:PHE:HB2 | 1:D:493:VAL:HG22 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:606:THR:C | 1:D:608:GLY:H | 2.22 | 0.42 |
| 3:F:1380:ILE:HD13 | 3:F:1458:TYR:CE1 | 2.54 | 0.42 |
| 3:F:1397:LYS:HA | 3:F:1400:ALA:HB3 | 2.00 | 0.42 |
| 1:A:427:VAL:CG2 | 1:A:523:GLU:HG3 | 2.50 | 0.42 |
| 3:C:1500:LYS:H | 3:C:1500:LYS:HG3 | 1.53 | 0.42 |
| 1:D:375:VAL:HG12 | 1:D:376:GLN:N | 2.34 | 0.42 |
| 1:D:439:LEU:HD12 | 1:D:439:LEU:N | 2.34 | 0.42 |
| 1:D:583:LEU:HD12 | 1:D:583:LEU:HA | 1.78 | 0.42 |
| 1:A:40:PHE:HA | 1:A:41:PRO:HA | 1.76 | 0.42 |
| 1:A:255:ASP:HA | 1:A:256:GLY:HA2 | 1.63 | 0.42 |
| 1:A:557:GLN:HG2 | 1:A:558:GLN:N | 2.35 | 0.42 |
| 3:C:1383:ILE:HB | 3:C:1422:LEU:HD23 | 2.01 | 0.42 |
| 3:C:1417:SER:OG | 3:C:1418:ASP:N | 2.52 | 0.42 |
| 3:C:1581:LEU:HD12 | 3:C:1582:MET:H | 1.80 | 0.42 |
| 3:C:1611:GLU:HG3 | 3:C:1612:GLU:H | 1.85 | 0.42 |
| 2:E:731:GLU:H | 2:E:731:GLU:HG3 | 1.66 | 0.42 |
| 3:F:1361:THR:HB | 3:F:1441:VAL:O | 2.19 | 0.42 |
| 3:F:1364:LEU:HD21 | 3:F:1471:TYR:OH | 2.20 | 0.42 |
| 3:F:1483:LEU:HD21 | 3:F:1590:TRP:CD1 | 2.55 | 0.42 |
| 3:F:1497:PHE:HD1 | 3:F:1606:VAL:HB | 1.85 | 0.42 |
| 3:F:1615:CYS:C | 3:F:1617:ASP:N | 2.72 | 0.42 |
| 1:A:138:GLY:O | 1:A:139:ARG:HG2 | 2.20 | 0.42 |
| 1:A:183:LYS:NZ | 1:A:185:ARG:CD | 2.82 | 0.42 |
| 1:A:183:LYS:HG2 | 1:A:199:GLU:HG2 | 2.01 | 0.42 |
| 2:B:841:ARG:HD3 | 2:B:861:GLN:HB2 | 2.01 | 0.42 |
| 3:C:1640:PRO:HB2 | 3:C:1641:ASN:H | 1.65 | 0.42 |
| 1:D:50:GLU:HG3 | 1:D:66:PHE:HB3 | 2.01 | 0.42 |
| 3:F:1403:VAL:HG22 | 3:F:1404:ASP:OD2 | 2.19 | 0.42 |
| 3:F:1536:PHE:O | 3:F:1536:PHE:CD1 | 2.73 | 0.42 |
| 3:F:1593:LYS:HA | 3:F:1596:LEU:HD21 | 2.00 | 0.42 |
| 1:A:386:LYS:O | 1:A:386:LYS:HG2 | 2.20 | 0.42 |
| 1:A:404:THR:HG23 | 1:A:415:ALA:N | 2.35 | 0.42 |
| 2:B:836:GLN:O | 2:B:836:GLN:HG3 | 2.19 | 0.42 |
| 3:C:1536:PHE:O | 3:C:1536:PHE:CD1 | 2.73 | 0.42 |
| 1:D:124:LEU:HA | 1:D:124:LEU:HD23 | 1.77 | 0.42 |
| 1:D:453:PHE:HB2 | 1:D:493:VAL:HG23 | 2.02 | 0.42 |
| 3:F:1462:ASN:HD21 | 3:F:1465:GLU:H | 1.66 | 0.42 |
| 3:F:1486:ASP:HB3 | 3:F:1487:GLU:H | 1.58 | 0.42 |
| 3:F:1513:LYS:C | 3:F:1515:CYS:N | 2.73 | 0.42 |
| 1:A:111:GLN:O | 1:A:125:TYR:HA | 2.19 | 0.42 |
| 1:A:255:ASP:OD1 | 1:A:300:LYS:HE3 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:760:PRO:O | 2:B:761:LYS:HG3 | 2.19 | 0.42 |
| 3:C:1344:THR:O | 3:C:1344:THR:HG22 | 2.19 | 0.42 |
| 3:C:1389:PHE:CE2 | 3:C:1443:GLN:CG | 2.99 | 0.42 |
| 3:C:1594:PRO:HD2 | 3:C:1595:ASN:ND2 | 2.34 | 0.42 |
| 1:D:456:ARG:HB2 | 1:D:456:ARG:NH1 | 2.35 | 0.42 |
| 1:D:469:THR:HG21 | 1:D:512:TYR:HE2 | 1.85 | 0.42 |
| 1:D:522:ARG:HB3 | 1:D:630:GLN:HE22 | 1.85 | 0.42 |
| 2:E:842:VAL:O | 2:E:861:GLN:HA | 2.20 | 0.42 |
| 3:F:1558:GLN:O | 3:F:1559:GLN:CB | 2.68 | 0.42 |
| 3:F:1611:GLU:HG3 | 3:F:1612:GLU:H | 1.85 | 0.42 |
| 4:H:72:LEU:O | 4:H:73:GLU:C | 2.58 | 0.42 |
| 1:A:64:VAL:O | 1:A:64:VAL:CG2 | 2.68 | 0.42 |
| 1:A:163:GLN:O | 1:A:164:LEU:HB3 | 2.20 | 0.42 |
| 1:A:369:VAL:CG1 | 1:A:400:ILE:HG22 | 2.50 | 0.42 |
| 3:C:1462:ASN:ND2 | 3:C:1464:GLU:OE1 | 2.53 | 0.42 |
| 1:D:153:VAL:O | 1:D:154:LYS:HB2 | 2.20 | 0.42 |
| 1:D:223:ILE:HD12 | 1:D:223:ILE:H | 1.83 | 0.42 |
| 1:D:404:THR:HG23 | 1:D:415:ALA:N | 2.35 | 0.42 |
| 3:F:1503:ASP:O | 3:F:1504:LYS:HB3 | 2.18 | 0.42 |
| 1:A:50:GLU:HG3 | 1:A:66:PHE:HB3 | 2.01 | 0.41 |
| 3:C:1485:ARG:HD3 | 3:C:1536:PHE:CE2 | 2.55 | 0.41 |
| 3:C:1639:CYS:O | 3:C:1640:PRO:C | 2.58 | 0.41 |
| 1:D:138:GLY:O | 1:D:139:ARG:HG2 | 2.20 | 0.41 |
| 1:D:338:THR:HG23 | 1:D:339:PRO:HD2 | 2.02 | 0.41 |
| 1:D:557:GLN:HG2 | 1:D:558:GLN:N | 2.35 | 0.41 |
| 2:E:894:VAL:HG11 | 2:E:899:ILE:HB | 2.00 | 0.41 |
| 2:E:910:VAL:CG2 | 2:E:911:PRO:HD2 | 2.47 | 0.41 |
| 3:F:1381:LEU:CD1 | 3:F:1437:LEU:HD21 | 2.49 | 0.41 |
| 3:F:1594:PRO:HD2 | 3:F:1595:ASN:ND2 | 2.34 | 0.41 |
| 1:A:56:PRO:HG3 | 1:A:60:HIS:CE1 | 2.56 | 0.41 |
| 1:A:368:ALA:HB2 | 1:A:376:GLN:HG2 | 2.02 | 0.41 |
| 1:A:459:ARG:HA | 1:A:462:GLU:HG2 | 2.01 | 0.41 |
| 3:C:1339:PHE:HA | 3:C:1369:ARG:O | 2.19 | 0.41 |
| 3:C:1367:CYS:C | 3:C:1434:ASP:OD2 | 2.58 | 0.41 |
| 1:D:356:ASN:HB3 | 1:D:357:PRO:CD | 2.50 | 0.41 |
| 1:D:365:VAL:H | 1:D:379:THR:CG2 | 2.33 | 0.41 |
| 1:D:369:VAL:CG1 | 1:D:400:ILE:HG22 | 2.50 | 0.41 |
| 1:D:495:LEU:HD12 | 1:D:496:PRO:HD2 | 2.02 | 0.41 |
| 2:E:750:LEU:C | 2:E:752:ASN:HD22 | 2.24 | 0.41 |
| 2:B:733:ILE:HB | 2:B:895:TYR:CD2 | 2.55 | 0.41 |
| 1:D:163:GLN:O | 1:D:164:LEU:HB3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:193:GLN:H | 1:D:193:GLN:CD | 2.23 | 0.41 |
| 3:F:1369:ARG:CG | 3:F:1370:TYR:N | 2.82 | 0.41 |
| 3:F:1579:HIS:CD2 | 3:F:1611:GLU:OE2 | 2.74 | 0.41 |
| 1:A:248:PHE:HD1 | 3:C:1378:MET:CE | 2.33 | 0.41 |
| 2:B:777:ILE:HD12 | 2:B:808:PHE:CD1 | 2.55 | 0.41 |
| 3:C:1387:THR:N | 3:C:1450:ILE:HG23 | 2.35 | 0.41 |
| 1:D:56:PRO:HG3 | 1:D:60:HIS:CE1 | 2.55 | 0.41 |
| 1:D:427:VAL:CG2 | 1:D:523:GLU:HG3 | 2.50 | 0.41 |
| 1:D:594:ILE:O | 1:D:597:VAL:HB | 2.21 | 0.41 |
| 3:F:1408:SER:O | 3:F:1409:LYS:C | 2.58 | 0.41 |
| 3:F:1497:PHE:CD1 | 3:F:1606:VAL:CG2 | 3.03 | 0.41 |
| 4:G:77:LYS:O | 4:G:80:ASP:HB2 | 2.21 | 0.41 |
| 4:H:77:LYS:HE2 | 4:H:81:GLU:OE2 | 2.20 | 0.41 |
| 1:A:356:ASN:HB3 | 1:A:357:PRO:CD | 2.50 | 0.41 |
| 1:A:365:VAL:H | 1:A:379:THR:CG2 | 2.33 | 0.41 |
| 2:B:761:LYS:O | 2:B:762:ASN:CG | 2.58 | 0.41 |
| 1:D:12:LEU:HG | 1:D:99:VAL:HG11 | 2.02 | 0.41 |
| 1:D:189:GLU:O | 1:D:192:PRO:HD3 | 2.21 | 0.41 |
| 1:D:368:ALA:HB2 | 1:D:376:GLN:HG2 | 2.02 | 0.41 |
| 3:C:1485:ARG:HD2 | 3:C:1536:PHE:CZ | 2.56 | 0.41 |
| 3:C:1518:GLY:HA3 | 3:C:1585:LEU:HD22 | 2.02 | 0.41 |
| 3:C:1558:GLN:O | 3:C:1559:GLN:CB | 2.68 | 0.41 |
| 1:D:47:LEU:HG | 1:D:48:SER:N | 2.33 | 0.41 |
| 1:A:12:LEU:HG | 1:A:99:VAL:HG11 | 2.02 | 0.41 |
| 1:A:453:PHE:HB2 | 1:A:493:VAL:HG23 | 2.02 | 0.41 |
| 1:A:522:ARG:HB3 | 1:A:630:GLN:HE22 | 1.85 | 0.41 |
| 3:C:1376:ALA:H | 3:C:1429:VAL:CG2 | 2.34 | 0.41 |
| 3:C:1396:LEU:O | 3:C:1399:LEU:HB2 | 2.21 | 0.41 |
| 1:D:45:LEU:HD11 | 1:D:48:SER:HB3 | 2.01 | 0.41 |
| 1:D:64:VAL:O | 1:D:64:VAL:CG2 | 2.68 | 0.41 |
| 1:D:444:ARG:HG3 | 1:D:444:ARG:HH11 | 1.86 | 0.41 |
| 1:A:45:LEU:HD11 | 1:A:48:SER:HB3 | 2.01 | 0.41 |
| 1:A:594:ILE:O | 1:A:597:VAL:HB | 2.21 | 0.41 |
| 2:E:750:LEU:HD11 | 2:E:769:MET:CE | 2.51 | 0.41 |
| 2:E:840:VAL:HG22 | 2:E:894:VAL:HB | 2.03 | 0.41 |
| 1:A:153:VAL:O | 1:A:154:LYS:HB2 | 2.20 | 0.41 |
| 1:A:189:GLU:O | 1:A:192:PRO:HD3 | 2.21 | 0.41 |
| 1:A:342:PHE:CE2 | 1:A:398:LEU:HB2 | 2.56 | 0.41 |
| 1:A:444:ARG:HG3 | 1:A:444:ARG:HH11 | 1.86 | 0.41 |
| 1:A:469:THR:HG21 | 1:A:512:TYR:HE2 | 1.85 | 0.41 |
| 1:A:495:LEU:HD12 | 1:A:496:PRO:HD2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:585:LYS:HB3 | 1:A:585:LYS:HE3 | 1.91 | 0.41 |
| 3:C:1341:LEU:CD1 | 3:C:1368:THR:HB | 2.44 | 0.41 |
| 3:C:1363:ILE:O | 3:C:1363:ILE:HG22 | 2.20 | 0.41 |
| 3:C:1472:HIS:HE1 | 3:C:1474:GLU:HG2 | 1.86 | 0.41 |
| 3:C:1579:HIS:CD2 | 3:C:1611:GLU:OE2 | 2.74 | 0.41 |
| 1:D:177:VAL:HG22 | 1:D:178:ASN:H | 1.85 | 0.41 |
| 1:D:517:GLY:O | 1:D:518:ALA:O | 2.38 | 0.41 |
| 3:F:1335:THR:O | 3:F:1336:CYS:CB | 2.65 | 0.41 |
| 3:F:1397:LYS:N | 3:F:1397:LYS:CD | 2.80 | 0.41 |
| 3:F:1460:TYR:O | 3:F:1462:ASN:N | 2.52 | 0.41 |
| 3:F:1506:THR:OG1 | 3:F:1507:LEU:N | 2.52 | 0.41 |
| 3:F:1518:GLY:HA3 | 3:F:1585:LEU:HD22 | 2.03 | 0.41 |
| 3:F:1591:GLY:CA | 3:F:1596:LEU:HB3 | 2.51 | 0.41 |
| 1:A:160:SER:C | 1:A:163:GLN:HB2 | 2.42 | 0.41 |
| 1:A:513:TYR:CZ | 1:A:525:VAL:HG11 | 2.56 | 0.41 |
| 3:C:1483:LEU:HD12 | 3:C:1483:LEU:HA | 1.89 | 0.41 |
| 1:D:107:TYR:CE2 | 1:D:132:HIS:HA | 2.56 | 0.41 |
| 1:D:204:GLU:OE1 | 2:E:815:TYR:CE2 | 2.72 | 0.41 |
| 1:D:253:ILE:HD12 | 1:D:302:LEU:HD23 | 1.95 | 0.41 |
| 1:D:255:ASP:OD1 | 1:D:300:LYS:HE3 | 2.20 | 0.41 |
| 1:D:312:SER:HB2 | 2:E:873:SER:OG | 2.21 | 0.41 |
| 3:F:1368:THR:HG22 | 3:F:1435:ASP:O | 2.21 | 0.41 |
| 3:F:1497:PHE:CG | 3:F:1498:ILE:N | 2.87 | 0.41 |
| 4:G:41:TYR:HD2 | 4:G:42:TYR:CD2 | 2.38 | 0.41 |
| 4:H:77:LYS:O | 4:H:80:ASP:HB2 | 2.21 | 0.41 |
| 3:C:1380:ILE:HG23 | 3:C:1423:ILE:CG2 | 2.29 | 0.40 |
| 3:C:1472:HIS:HE1 | 3:C:1474:GLU:CG | 2.33 | 0.40 |
| 1:D:63:ASN:C | 1:D:64:VAL:HG13 | 2.37 | 0.40 |
| 4:G:77:LYS:HE2 | 4:G:81:GLU:OE2 | 2.20 | 0.40 |
| 4:H:41:TYR:HD2 | 4:H:42:TYR:CD2 | 2.38 | 0.40 |
| 1:A:35:VAL:HG22 | 1:A:88:ALA:CB | 2.51 | 0.40 |
| 1:A:107:TYR:CE2 | 1:A:132:HIS:HA | 2.56 | 0.40 |
| 2:B:855:THR:HB | 3:C:1602:LYS:HZ2 | 1.87 | 0.40 |
| 3:C:1360:ASN:HD22 | 3:C:1362:MET:CE | 2.34 | 0.40 |
| 1:D:6:ILE:HA | 1:D:6:ILE:HD12 | 1.68 | 0.40 |
| 1:D:35:VAL:HG22 | 1:D:88:ALA:CB | 2.51 | 0.40 |
| 1:D:151:ILE:HG22 | 1:D:153:VAL:HG12 | 2.03 | 0.40 |
| 1:D:407:GLN:C | 1:D:409:LEU:H | 2.24 | 0.40 |
| 3:F:1591:GLY:O | 3:F:1596:LEU:HB3 | 2.22 | 0.40 |
| 1:A:177:VAL:HG22 | 1:A:178:ASN:H | 1.85 | 0.40 |
| 1:A:193:GLN:H | 1:A:193:GLN:CD | 2.24 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:346:MET:HE1 | 1:A:456:ARG:CB | 2.40 | 0.40 |
| 1:A:517:GLY:O | 1:A:518:ALA:O | 2.38 | 0.40 |
| 1:A:544:LYS:HG3 | 1:A:562:LYS:HB3 | 2.02 | 0.40 |
| 2:B:895:TYR:O | 2:B:897:HIS:N | 2.44 | 0.40 |
| 3:C:1512:ASP:O | 3:C:1515:CYS:N | 2.52 | 0.40 |
| 3:C:1516:GLU:HB3 | 3:C:1517:PRO:CD | 2.51 | 0.40 |
| 1:D:48:SER:C | 1:D:49:SER:O | 2.60 | 0.40 |
| 1:D:338:THR:HG21 | 1:D:419:MET:HE1 | 2.02 | 0.40 |
| 1:D:341:TYR:HA | 1:D:422:LEU:O | 2.21 | 0.40 |
| 2:E:778:THR:OG1 | 2:E:779:THR:N | 2.54 | 0.40 |
| 3:F:1504:LYS:HD3 | 3:F:1504:LYS:N | 2.37 | 0.40 |
| 3:F:1566:ILE:C | 3:F:1568:CYS:N | 2.75 | 0.40 |
| 4:H:18:ALA:N | 4:H:65:MET:HE1 | 2.34 | 0.40 |
| 1:A:226:GLU:HA | 1:A:282:ARG:HD2 | 2.03 | 0.40 |
| 2:B:758:GLU:O | 2:B:759:PRO:C | 2.60 | 0.40 |
| 2:B:830:TYR:CD1 | 2:B:871:SER:HB3 | 2.56 | 0.40 |
| 3:C:1472:HIS:CD2 | 3:C:1475:LYS:HD2 | 2.57 | 0.40 |
| 1:D:342:PHE:CE2 | 1:D:398:LEU:HB2 | 2.56 | 0.40 |
| 1:D:346:MET:CG | 1:D:347:PRO:HD2 | 2.51 | 0.40 |
| 1:D:386:LYS:O | 1:D:386:LYS:HG2 | 2.20 | 0.40 |
| 1:D:563:ILE:O | 2:E:766:THR:HA | 2.22 | 0.40 |
| 1:A:530:TRP:CZ3 | 1:A:532:ASP:HB2 | 2.56 | 0.40 |
| 3:C:1411:GLU:CD | 3:C:1422:LEU:HA | 2.42 | 0.40 |
| 1:D:183:LYS:NZ | 1:D:185:ARG:CD | 2.82 | 0.40 |
| 1:D:471:LEU:HB3 | 1:D:478:LEU:HD21 | 2.04 | 0.40 |
| 3:F:1450:ILE:CD1 | 3:F:1472:HIS:CE1 | 2.96 | 0.40 |
| 3:F:1622:LYS:HD2 | 3:F:1622:LYS:HA | 1.55 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1 | A | 629/645 (98%) | 553 (88%) | 57 (9%) | 19 (3%) | 4 | 23 |
| 1 | D | 629/645 (98%) | 548 (87%) | 62 (10%) | 19 (3%) | 4 | 23 |
| 2 | B | 181/206 (88%) | 157 (87%) | 18 (10%) | 6 (3%) | 4 | 22 |
| 2 | E | 181/206 (88%) | 157 (87%) | 19 (10%) | 5 (3%) | 5 | 24 |
| 3 | C | 290/343 (84%) | 226 (78%) | 42 (14%) | 22 (8%) | 1 | 6 |
| 3 | F | 290/343 (84%) | 213 (73%) | 48 (17%) | 29 (10%) | 0 | 4 |
| 4 | G | 66/73 (90%) | 56 (85%) | 10 (15%) | 0 | 100 | 100 |
| 4 | H | 66/73 (90%) | 55 (83%) | 11 (17%) | 0 | 100 | 100 |
| All | All | 2332/2534 (92%) | 1965 (84%) | 267 (11%) | 100 (4%) | 2 | 17 |

All (100) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 49 | SER |
| 1 | A | 347 | PRO |
| 1 | A | 392 | HIS |
| 1 | A | 518 | ALA |
| 1 | A | 549 | GLU |
| 2 | B | 836 | GLN |
| 3 | C | 1361 | THR |
| 3 | C | 1417 | SER |
| 3 | C | 1434 | ASP |
| 3 | C | 1477 | ASP |
| 3 | C | 1496 | CYS |
| 3 | C | 1640 | PRO |
| 1 | D | 49 | SER |
| 1 | D | 292 | PRO |
| 1 | D | 518 | ALA |
| 1 | D | 549 | GLU |
| 2 | E | 836 | GLN |
| 3 | F | 1375 | ASP |
| 3 | F | 1402 | GLY |
| 3 | F | 1412 | LEU |
| 3 | F | 1415 | ALA |
| 3 | F | 1481 | ASN |
| 3 | F | 1496 | CYS |
| 3 | F | 1499 | GLN |
| 3 | F | 1556 | VAL |
| 1 | A | 59 | ASN |
| 1 | A | 574 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | B | 762 | ASN |
| 3 | C | 1366 | ILE |
| 3 | C | 1367 | CYS |
| 3 | C | 1402 | GLY |
| 3 | C | 1486 | ASP |
| 3 | C | 1504 | LYS |
| 3 | C | 1512 | ASP |
| 3 | C | 1528 | VAL |
| 1 | D | 59 | ASN |
| 1 | D | 551 | ARG |
| 1 | D | 574 | VAL |
| 3 | F | 1361 | THR |
| 3 | F | 1461 | TYR |
| 3 | F | 1492 | ALA |
| 3 | F | 1504 | LYS |
| 3 | F | 1512 | ASP |
| 3 | F | 1528 | VAL |
| 1 | A | 63 | ASN |
| 1 | A | 64 | VAL |
| 1 | A | 372 | GLU |
| 1 | A | 548 | SER |
| 2 | B | 835 | ASN |
| 2 | B | 869 | LYS |
| 3 | C | 1392 | ASP |
| 3 | C | 1412 | LEU |
| 3 | C | 1494 | GLU |
| 3 | C | 1513 | LYS |
| 3 | C | 1602 | LYS |
| 1 | D | 63 | ASN |
| 1 | D | 64 | VAL |
| 1 | D | 372 | GLU |
| 2 | E | 762 | ASN |
| 2 | E | 835 | ASN |
| 2 | E | 869 | LYS |
| 3 | F | 1336 | CYS |
| 3 | F | 1449 | LEU |
| 3 | F | 1462 | ASN |
| 3 | F | 1513 | LYS |
| 3 | F | 1602 | LYS |
| 3 | F | 1616 | GLN |
| 1 | A | 375 | VAL |
| 1 | A | 376 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 732 | ASP |
| 3 | C | 1505 | VAL |
| 3 | C | 1559 | GLN |
| 1 | D | 375 | VAL |
| 1 | D | 376 | GLN |
| 2 | E | 732 | ASP |
| 3 | F | 1387 | THR |
| 3 | F | 1493 | GLU |
| 3 | F | 1505 | VAL |
| 3 | F | 1514 | ALA |
| 3 | F | 1559 | GLN |
| 3 | F | 1640 | PRO |
| 1 | A | 81 | ASN |
| 1 | A | 506 | SER |
| 1 | A | 607 | PRO |
| 2 | B | 759 | PRO |
| 1 | D | 81 | ASN |
| 1 | D | 506 | SER |
| 1 | D | 607 | PRO |
| 3 | F | 1393 | THR |
| 1 | A | 539 | GLY |
| 3 | C | 1393 | THR |
| 1 | D | 539 | GLY |
| 1 | D | 553 | PRO |
| 3 | C | 1547 | ILE |
| 3 | F | 1547 | ILE |
| 1 | A | 91 | GLY |
| 1 | A | 520 | GLY |
| 1 | D | 520 | GLY |
| 3 | F | 1391 | PRO |
| 1 | D | 91 | GLY |

5.3.2 Protein sidechains [i](#)

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.

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1 | A | 558/567 (98%) | 476 (85%) | 82 (15%) | 3 | 12 |
| 1 | D | 558/567 (98%) | 474 (85%) | 84 (15%) | 3 | 12 |
| 2 | B | 171/191 (90%) | 155 (91%) | 16 (9%) | 8 | 30 |
| 2 | E | 171/191 (90%) | 154 (90%) | 17 (10%) | 8 | 27 |
| 3 | C | 270/309 (87%) | 218 (81%) | 52 (19%) | 1 | 4 |
| 3 | F | 270/309 (87%) | 204 (76%) | 66 (24%) | 0 | 2 |
| 4 | G | 57/60 (95%) | 54 (95%) | 3 (5%) | 22 | 52 |
| 4 | H | 57/60 (95%) | 53 (93%) | 4 (7%) | 15 | 44 |
| All | All | 2112/2254 (94%) | 1788 (85%) | 324 (15%) | 2 | 11 |

All (324) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 6 | ILE |
| 1 | A | 20 | MET |
| 1 | A | 31 | VAL |
| 1 | A | 34 | THR |
| 1 | A | 45 | LEU |
| 1 | A | 46 | VAL |
| 1 | A | 47 | LEU |
| 1 | A | 58 | THR |
| 1 | A | 61 | MET |
| 1 | A | 80 | ARG |
| 1 | A | 87 | GLN |
| 1 | A | 92 | THR |
| 1 | A | 94 | VAL |
| 1 | A | 102 | SER |
| 1 | A | 112 | THR |
| 1 | A | 118 | THR |
| 1 | A | 134 | LEU |
| 1 | A | 137 | VAL |
| 1 | A | 139 | ARG |
| 1 | A | 145 | ILE |
| 1 | A | 155 | GLN |
| 1 | A | 161 | GLN |
| 1 | A | 163 | GLN |
| 1 | A | 164 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 172 | ASP |
| 1 | A | 179 | MET |
| 1 | A | 183 | LYS |
| 1 | A | 195 | VAL |
| 1 | A | 198 | THR |
| 1 | A | 207 | LEU |
| 1 | A | 214 | VAL |
| 1 | A | 215 | GLU |
| 1 | A | 223 | ILE |
| 1 | A | 226 | GLU |
| 1 | A | 249 | VAL |
| 1 | A | 257 | GLU |
| 1 | A | 261 | SER |
| 1 | A | 263 | PRO |
| 1 | A | 264 | GLU |
| 1 | A | 277 | GLU |
| 1 | A | 293 | ARG |
| 1 | A | 304 | VAL |
| 1 | A | 305 | SER |
| 1 | A | 326 | ILE |
| 1 | A | 329 | SER |
| 1 | A | 364 | ARG |
| 1 | A | 369 | VAL |
| 1 | A | 370 | GLN |
| 1 | A | 373 | ASP |
| 1 | A | 379 | THR |
| 1 | A | 380 | GLN |
| 1 | A | 398 | LEU |
| 1 | A | 400 | ILE |
| 1 | A | 404 | THR |
| 1 | A | 406 | LYS |
| 1 | A | 409 | LEU |
| 1 | A | 417 | ARG |
| 1 | A | 419 | MET |
| 1 | A | 426 | THR |
| 1 | A | 443 | LEU |
| 1 | A | 448 | THR |
| 1 | A | 454 | LEU |
| 1 | A | 456 | ARG |
| 1 | A | 462 | GLU |
| 1 | A | 477 | ARG |
| 1 | A | 485 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 487 | GLU |
| 1 | A | 492 | LEU |
| 1 | A | 509 | LEU |
| 1 | A | 510 | VAL |
| 1 | A | 519 | SER |
| 1 | A | 535 | ASP |
| 1 | A | 542 | VAL |
| 1 | A | 558 | GLN |
| 1 | A | 559 | MET |
| 1 | A | 561 | LEU |
| 1 | A | 583 | LEU |
| 1 | A | 585 | LYS |
| 1 | A | 592 | SER |
| 1 | A | 609 | SER |
| 1 | A | 625 | THR |
| 1 | A | 639 | GLN |
| 2 | B | 730 | ASP |
| 2 | B | 731 | GLU |
| 2 | B | 732 | ASP |
| 2 | B | 764 | ILE |
| 2 | B | 765 | SER |
| 2 | B | 775 | ASP |
| 2 | B | 813 | LEU |
| 2 | B | 817 | VAL |
| 2 | B | 819 | ARG |
| 2 | B | 834 | GLN |
| 2 | B | 845 | LEU |
| 2 | B | 864 | VAL |
| 2 | B | 887 | GLU |
| 2 | B | 894 | VAL |
| 2 | B | 907 | LEU |
| 2 | B | 910 | VAL |
| 3 | C | 1335 | THR |
| 3 | C | 1342 | LYS |
| 3 | C | 1344 | THR |
| 3 | C | 1361 | THR |
| 3 | C | 1363 | ILE |
| 3 | C | 1366 | ILE |
| 3 | C | 1368 | THR |
| 3 | C | 1374 | GLN |
| 3 | C | 1385 | MET |
| 3 | C | 1393 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | C | 1395 | ASP |
| 3 | C | 1397 | LYS |
| 3 | C | 1404 | ASP |
| 3 | C | 1405 | ARG |
| 3 | C | 1411 | GLU |
| 3 | C | 1416 | PHE |
| 3 | C | 1422 | LEU |
| 3 | C | 1426 | LEU |
| 3 | C | 1433 | GLU |
| 3 | C | 1437 | LEU |
| 3 | C | 1443 | GLN |
| 3 | C | 1447 | VAL |
| 3 | C | 1457 | VAL |
| 3 | C | 1462 | ASN |
| 3 | C | 1469 | ARG |
| 3 | C | 1474 | GLU |
| 3 | C | 1477 | ASP |
| 3 | C | 1479 | LYS |
| 3 | C | 1480 | LEU |
| 3 | C | 1489 | CYS |
| 3 | C | 1494 | GLU |
| 3 | C | 1495 | ASN |
| 3 | C | 1499 | GLN |
| 3 | C | 1503 | ASP |
| 3 | C | 1504 | LYS |
| 3 | C | 1532 | LEU |
| 3 | C | 1535 | ASP |
| 3 | C | 1538 | GLU |
| 3 | C | 1543 | ILE |
| 3 | C | 1551 | SER |
| 3 | C | 1554 | VAL |
| 3 | C | 1558 | GLN |
| 3 | C | 1559 | GLN |
| 3 | C | 1564 | SER |
| 3 | C | 1567 | LYS |
| 3 | C | 1568 | CYS |
| 3 | C | 1573 | LYS |
| 3 | C | 1582 | MET |
| 3 | C | 1586 | SER |
| 3 | C | 1608 | HIS |
| 3 | C | 1624 | CYS |
| 3 | C | 1631 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | D | 6 | ILE |
| 1 | D | 20 | MET |
| 1 | D | 31 | VAL |
| 1 | D | 34 | THR |
| 1 | D | 45 | LEU |
| 1 | D | 46 | VAL |
| 1 | D | 47 | LEU |
| 1 | D | 58 | THR |
| 1 | D | 61 | MET |
| 1 | D | 80 | ARG |
| 1 | D | 87 | GLN |
| 1 | D | 92 | THR |
| 1 | D | 94 | VAL |
| 1 | D | 102 | SER |
| 1 | D | 112 | THR |
| 1 | D | 118 | THR |
| 1 | D | 134 | LEU |
| 1 | D | 137 | VAL |
| 1 | D | 139 | ARG |
| 1 | D | 145 | ILE |
| 1 | D | 155 | GLN |
| 1 | D | 161 | GLN |
| 1 | D | 163 | GLN |
| 1 | D | 164 | LEU |
| 1 | D | 172 | ASP |
| 1 | D | 179 | MET |
| 1 | D | 183 | LYS |
| 1 | D | 195 | VAL |
| 1 | D | 198 | THR |
| 1 | D | 207 | LEU |
| 1 | D | 214 | VAL |
| 1 | D | 215 | GLU |
| 1 | D | 223 | ILE |
| 1 | D | 226 | GLU |
| 1 | D | 249 | VAL |
| 1 | D | 257 | GLU |
| 1 | D | 261 | SER |
| 1 | D | 263 | PRO |
| 1 | D | 264 | GLU |
| 1 | D | 277 | GLU |
| 1 | D | 293 | ARG |
| 1 | D | 304 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | D | 305 | SER |
| 1 | D | 326 | ILE |
| 1 | D | 329 | SER |
| 1 | D | 364 | ARG |
| 1 | D | 369 | VAL |
| 1 | D | 370 | GLN |
| 1 | D | 373 | ASP |
| 1 | D | 379 | THR |
| 1 | D | 380 | GLN |
| 1 | D | 392 | HIS |
| 1 | D | 398 | LEU |
| 1 | D | 400 | ILE |
| 1 | D | 404 | THR |
| 1 | D | 406 | LYS |
| 1 | D | 409 | LEU |
| 1 | D | 417 | ARG |
| 1 | D | 419 | MET |
| 1 | D | 426 | THR |
| 1 | D | 443 | LEU |
| 1 | D | 448 | THR |
| 1 | D | 456 | ARG |
| 1 | D | 462 | GLU |
| 1 | D | 477 | ARG |
| 1 | D | 485 | VAL |
| 1 | D | 487 | GLU |
| 1 | D | 492 | LEU |
| 1 | D | 509 | LEU |
| 1 | D | 510 | VAL |
| 1 | D | 519 | SER |
| 1 | D | 535 | ASP |
| 1 | D | 542 | VAL |
| 1 | D | 547 | GLN |
| 1 | D | 551 | ARG |
| 1 | D | 558 | GLN |
| 1 | D | 559 | MET |
| 1 | D | 561 | LEU |
| 1 | D | 583 | LEU |
| 1 | D | 585 | LYS |
| 1 | D | 592 | SER |
| 1 | D | 609 | SER |
| 1 | D | 625 | THR |
| 1 | D | 639 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 2 | E | 730 | ASP |
| 2 | E | 731 | GLU |
| 2 | E | 732 | ASP |
| 2 | E | 757 | LYS |
| 2 | E | 764 | ILE |
| 2 | E | 775 | ASP |
| 2 | E | 813 | LEU |
| 2 | E | 817 | VAL |
| 2 | E | 819 | ARG |
| 2 | E | 834 | GLN |
| 2 | E | 845 | LEU |
| 2 | E | 851 | CYS |
| 2 | E | 864 | VAL |
| 2 | E | 887 | GLU |
| 2 | E | 894 | VAL |
| 2 | E | 907 | LEU |
| 2 | E | 910 | VAL |
| 3 | F | 1335 | THR |
| 3 | F | 1342 | LYS |
| 3 | F | 1344 | THR |
| 3 | F | 1346 | LYS |
| 3 | F | 1361 | THR |
| 3 | F | 1363 | ILE |
| 3 | F | 1364 | LEU |
| 3 | F | 1366 | ILE |
| 3 | F | 1371 | ARG |
| 3 | F | 1373 | ASP |
| 3 | F | 1374 | GLN |
| 3 | F | 1377 | THR |
| 3 | F | 1378 | MET |
| 3 | F | 1385 | MET |
| 3 | F | 1387 | THR |
| 3 | F | 1393 | THR |
| 3 | F | 1395 | ASP |
| 3 | F | 1397 | LYS |
| 3 | F | 1398 | GLN |
| 3 | F | 1404 | ASP |
| 3 | F | 1411 | GLU |
| 3 | F | 1412 | LEU |
| 3 | F | 1417 | SER |
| 3 | F | 1418 | ASP |
| 3 | F | 1422 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 3 | F | 1423 | ILE |
| 3 | F | 1428 | LYS |
| 3 | F | 1432 | SER |
| 3 | F | 1433 | GLU |
| 3 | F | 1434 | ASP |
| 3 | F | 1436 | CYS |
| 3 | F | 1440 | LYS |
| 3 | F | 1449 | LEU |
| 3 | F | 1457 | VAL |
| 3 | F | 1462 | ASN |
| 3 | F | 1469 | ARG |
| 3 | F | 1474 | GLU |
| 3 | F | 1479 | LYS |
| 3 | F | 1482 | LYS |
| 3 | F | 1483 | LEU |
| 3 | F | 1490 | ARG |
| 3 | F | 1491 | CYS |
| 3 | F | 1497 | PHE |
| 3 | F | 1499 | GLN |
| 3 | F | 1503 | ASP |
| 3 | F | 1504 | LYS |
| 3 | F | 1532 | LEU |
| 3 | F | 1535 | ASP |
| 3 | F | 1538 | GLU |
| 3 | F | 1543 | ILE |
| 3 | F | 1551 | SER |
| 3 | F | 1554 | VAL |
| 3 | F | 1558 | GLN |
| 3 | F | 1559 | GLN |
| 3 | F | 1564 | SER |
| 3 | F | 1567 | LYS |
| 3 | F | 1573 | LYS |
| 3 | F | 1582 | MET |
| 3 | F | 1586 | SER |
| 3 | F | 1596 | LEU |
| 3 | F | 1608 | HIS |
| 3 | F | 1616 | GLN |
| 3 | F | 1622 | LYS |
| 3 | F | 1624 | CYS |
| 3 | F | 1631 | THR |
| 3 | F | 1639 | CYS |
| 4 | G | 25 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 4 | G | 33 | LEU |
| 4 | G | 37 | SER |
| 4 | H | 25 | LEU |
| 4 | H | 33 | LEU |
| 4 | H | 37 | SER |
| 4 | H | 64 | SER |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 10 | ASN |
| 1 | A | 38 | HIS |
| 1 | A | 60 | HIS |
| 1 | A | 87 | GLN |
| 1 | A | 104 | GLN |
| 1 | A | 132 | HIS |
| 1 | A | 193 | GLN |
| 1 | A | 318 | GLN |
| 1 | A | 332 | GLN |
| 1 | A | 395 | GLN |
| 1 | A | 429 | ASN |
| 1 | A | 490 | GLN |
| 1 | A | 634 | GLN |
| 1 | A | 639 | GLN |
| 2 | B | 738 | ASN |
| 2 | B | 752 | ASN |
| 2 | B | 770 | ASN |
| 2 | B | 834 | GLN |
| 2 | B | 836 | GLN |
| 2 | B | 897 | HIS |
| 3 | C | 1360 | ASN |
| 3 | C | 1443 | GLN |
| 3 | C | 1446 | ASN |
| 3 | C | 1462 | ASN |
| 3 | C | 1481 | ASN |
| 3 | C | 1495 | ASN |
| 3 | C | 1579 | HIS |
| 3 | C | 1595 | ASN |
| 1 | D | 10 | ASN |
| 1 | D | 38 | HIS |
| 1 | D | 60 | HIS |
| 1 | D | 87 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 104 | GLN |
| 1 | D | 132 | HIS |
| 1 | D | 155 | GLN |
| 1 | D | 181 | GLN |
| 1 | D | 193 | GLN |
| 1 | D | 290 | GLN |
| 1 | D | 291 | ASN |
| 1 | D | 318 | GLN |
| 1 | D | 332 | GLN |
| 1 | D | 395 | GLN |
| 1 | D | 429 | ASN |
| 1 | D | 490 | GLN |
| 1 | D | 634 | GLN |
| 1 | D | 639 | GLN |
| 2 | E | 738 | ASN |
| 2 | E | 752 | ASN |
| 2 | E | 762 | ASN |
| 2 | E | 770 | ASN |
| 2 | E | 820 | ASN |
| 2 | E | 834 | GLN |
| 2 | E | 836 | GLN |
| 2 | E | 860 | HIS |
| 2 | E | 897 | HIS |
| 3 | F | 1337 | ASN |
| 3 | F | 1401 | ASN |
| 3 | F | 1462 | ASN |
| 3 | F | 1499 | GLN |
| 3 | F | 1559 | GLN |
| 3 | F | 1579 | HIS |
| 3 | F | 1595 | ASN |
| 3 | F | 1641 | ASN |

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 | 633/645 (98%) | 0.05 | 12 (1%) 66 65 | 25, 50, 86, 148 | 0 |
| 1 | D | 633/645 (98%) | 0.00 | 4 (0%) 89 89 | 21, 53, 85, 141 | 0 |
| 2 | B | 183/206 (88%) | -0.16 | 1 (0%) 91 90 | 27, 54, 93, 121 | 0 |
| 2 | E | 183/206 (88%) | -0.22 | 3 (1%) 72 70 | 26, 48, 76, 126 | 0 |
| 3 | C | 296/343 (86%) | 1.32 | 65 (21%) 0 1 | 24, 116, 155, 187 | 0 |
| 3 | F | 296/343 (86%) | 0.73 | 27 (9%) 9 10 | 26, 90, 126, 147 | 0 |
| 4 | G | 68/73 (93%) | 0.06 | 1 (1%) 73 72 | 35, 59, 106, 115 | 0 |
| 4 | H | 68/73 (93%) | -0.20 | 0 100 100 | 36, 47, 67, 79 | 0 |
| All | All | 2360/2534 (93%) | 0.24 | 113 (4%) 30 31 | 21, 59, 127, 187 | 0 |

All (113) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | C | 1500 | LYS | 7.2 |
| 3 | F | 1641 | ASN | 6.9 |
| 3 | C | 1503 | ASP | 6.4 |
| 3 | C | 1415 | ALA | 5.5 |
| 3 | C | 1606 | VAL | 4.8 |
| 3 | C | 1499 | GLN | 4.7 |
| 3 | C | 1412 | LEU | 4.5 |
| 3 | C | 1497 | PHE | 4.2 |
| 3 | F | 1594 | PRO | 4.0 |
| 3 | C | 1445 | PHE | 4.0 |
| 3 | F | 1500 | LYS | 4.0 |
| 3 | C | 1349 | PRO | 3.8 |
| 3 | F | 1503 | ASP | 3.6 |
| 3 | C | 1605 | TRP | 3.6 |
| 3 | C | 1608 | HIS | 3.6 |
| 2 | E | 763 | GLY | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 3 | C | 1583 | TRP | 3.5 |
| 3 | C | 1364 | LEU | 3.4 |
| 3 | C | 1534 | ASN | 3.4 |
| 1 | A | 291 | ASN | 3.4 |
| 1 | A | 292 | PRO | 3.3 |
| 3 | F | 1359 | LYS | 3.3 |
| 1 | A | 373 | ASP | 3.3 |
| 3 | F | 1536 | PHE | 3.2 |
| 3 | F | 1506 | THR | 3.2 |
| 3 | C | 1416 | PHE | 3.1 |
| 3 | C | 1641 | ASN | 3.1 |
| 3 | C | 1368 | THR | 3.1 |
| 3 | C | 1581 | LEU | 3.1 |
| 3 | F | 1499 | GLN | 3.1 |
| 3 | C | 1498 | ILE | 3.1 |
| 3 | C | 1487 | GLU | 3.1 |
| 3 | C | 1609 | TRP | 3.1 |
| 3 | C | 1582 | MET | 3.1 |
| 1 | D | 551 | ARG | 3.1 |
| 3 | C | 1439 | PHE | 3.0 |
| 3 | C | 1553 | GLU | 3.0 |
| 3 | F | 1504 | LYS | 2.9 |
| 3 | C | 1545 | GLN | 2.9 |
| 3 | C | 1441 | VAL | 2.9 |
| 3 | C | 1574 | LEU | 2.9 |
| 3 | C | 1520 | ASP | 2.8 |
| 3 | C | 1446 | ASN | 2.8 |
| 4 | G | 67 | ASP | 2.8 |
| 3 | F | 1416 | PHE | 2.8 |
| 3 | C | 1571 | ALA | 2.8 |
| 3 | C | 1419 | ARG | 2.8 |
| 3 | C | 1570 | GLU | 2.8 |
| 1 | D | 294 | ALA | 2.8 |
| 3 | C | 1372 | GLY | 2.7 |
| 3 | F | 1505 | VAL | 2.7 |
| 3 | C | 1426 | LEU | 2.7 |
| 3 | F | 1566 | ILE | 2.7 |
| 3 | C | 1381 | LEU | 2.7 |
| 3 | C | 1561 | THR | 2.7 |
| 3 | F | 1606 | VAL | 2.6 |
| 3 | F | 1412 | LEU | 2.6 |
| 3 | F | 1534 | ASN | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | C | 1623 | GLN | 2.6 |
| 3 | C | 1382 | ASP | 2.6 |
| 2 | E | 762 | ASN | 2.6 |
| 2 | E | 765 | SER | 2.5 |
| 3 | C | 1639 | CYS | 2.5 |
| 3 | F | 1349 | PRO | 2.5 |
| 3 | F | 1595 | ASN | 2.5 |
| 3 | F | 1582 | MET | 2.5 |
| 1 | A | 374 | THR | 2.4 |
| 3 | C | 1629 | ALA | 2.4 |
| 1 | A | 289 | VAL | 2.4 |
| 3 | C | 1454 | ALA | 2.4 |
| 3 | C | 1443 | GLN | 2.4 |
| 3 | C | 1505 | VAL | 2.3 |
| 3 | F | 1640 | PRO | 2.3 |
| 3 | C | 1424 | ILE | 2.3 |
| 3 | F | 1585 | LEU | 2.3 |
| 3 | C | 1495 | ASN | 2.3 |
| 3 | C | 1523 | TYR | 2.3 |
| 3 | F | 1564 | SER | 2.3 |
| 3 | C | 1343 | VAL | 2.3 |
| 1 | D | 552 | GLN | 2.3 |
| 3 | C | 1584 | GLY | 2.3 |
| 3 | C | 1612 | GLU | 2.3 |
| 1 | A | 105 | SER | 2.3 |
| 3 | C | 1444 | TYR | 2.3 |
| 3 | C | 1373 | ASP | 2.3 |
| 3 | C | 1531 | GLN | 2.2 |
| 1 | A | 48 | SER | 2.2 |
| 3 | C | 1432 | SER | 2.2 |
| 1 | A | 548 | SER | 2.2 |
| 3 | C | 1632 | GLU | 2.2 |
| 3 | C | 1423 | ILE | 2.2 |
| 3 | C | 1504 | LYS | 2.2 |
| 2 | B | 763 | GLY | 2.2 |
| 1 | A | 80 | ARG | 2.1 |
| 3 | C | 1638 | GLY | 2.1 |
| 3 | F | 1518 | GLY | 2.1 |
| 1 | D | 30 | ASP | 2.1 |
| 1 | A | 371 | GLY | 2.1 |
| 3 | F | 1360 | ASN | 2.1 |
| 3 | F | 1364 | LEU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 3 | C | 1488 | LEU | 2.1 |
| 3 | C | 1590 | TRP | 2.1 |
| 3 | C | 1580 | TYR | 2.1 |
| 3 | C | 1597 | SER | 2.1 |
| 3 | C | 1575 | GLU | 2.0 |
| 3 | C | 1468 | THR | 2.0 |
| 1 | A | 106 | GLY | 2.0 |
| 3 | C | 1557 | GLY | 2.0 |
| 3 | F | 1439 | PHE | 2.0 |
| 3 | F | 1443 | GLN | 2.0 |
| 3 | C | 1596 | LEU | 2.0 |
| 3 | F | 1398 | GLN | 2.0 |
| 1 | A | 229 | LEU | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.