



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:34 AM GMT

PDB ID : 3F3G
Title : Crystal structure of the nucleoporin pair Nup85-Seh1, space group P212121
Authors : Debler, E.W.; Hseo, H.; Ma, Y.; Blobel, G.; Hoelz, A.
Deposited on : 2008-10-30
Resolution : 3.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

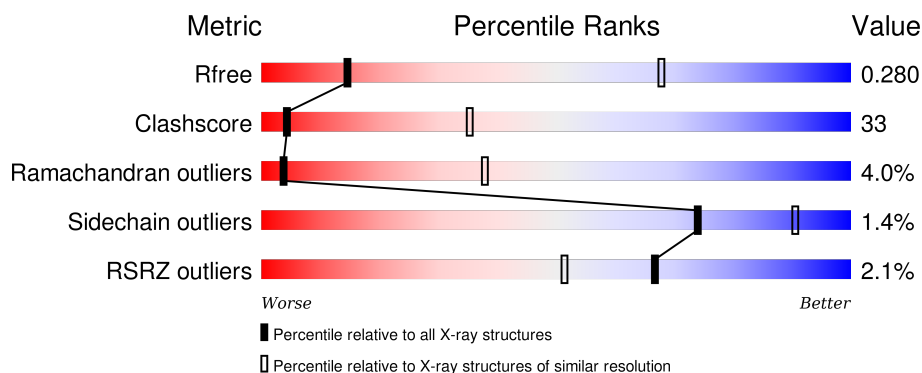
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 1268 (4.02-3.50) |
| Clashscore | 102246 | 1407 (4.02-3.50) |
| Ramachandran outliers | 100387 | 1346 (4.02-3.50) |
| Sidechain outliers | 100360 | 1342 (4.02-3.50) |
| RSRZ outliers | 91569 | 1276 (4.02-3.50) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 351 | <div> <div>2%</div> <div> <div></div> <div>41%</div> <div>43%</div> <div>•</div> <div>15%</div> </div> </div> |
| 1 | B | 351 | <div> <div>2%</div> <div> <div></div> <div>38%</div> <div>45%</div> <div>•</div> <div>15%</div> </div> </div> |
| 1 | E | 351 | <div> <div>3%</div> <div> <div></div> <div>38%</div> <div>45%</div> <div>•</div> <div>15%</div> </div> </div> |
| 1 | F | 351 | <div> <div>3%</div> <div> <div></div> <div>40%</div> <div>43%</div> <div>•</div> <div>15%</div> </div> </div> |
| 2 | C | 570 | <div> <div>2%</div> <div> <div></div> <div>39%</div> <div>43%</div> <div>•</div> <div>14%</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | D | 570 | <div><div><div>%</div><div><div></div><div></div><div></div></div><div>39%42%16%</div></div></div> |
| 2 | G | 570 | <div><div><div>%</div><div><div></div><div></div><div></div></div><div>40%41%15%</div></div></div> |
| 2 | H | 570 | <div><div><div>%</div><div><div></div><div></div><div></div></div><div>39%43%14%</div></div></div> |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25114 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 Nucleoporin SEH1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 300 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2379 | 1506 | 410 | 452 | 11 | | | |
| 1 | B | 300 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2379 | 1506 | 410 | 452 | 11 | | | |
| 1 | E | 300 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2379 | 1506 | 410 | 452 | 11 | | | |
| 1 | F | 300 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2379 | 1506 | 410 | 452 | 11 | | | |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | -1 | PRO | - | EXPRESSION TAG | UNP P53011 |
| A | 0 | HIS | - | EXPRESSION TAG | UNP P53011 |
| B | -1 | PRO | - | EXPRESSION TAG | UNP P53011 |
| B | 0 | HIS | - | EXPRESSION TAG | UNP P53011 |
| E | -1 | PRO | - | EXPRESSION TAG | UNP P53011 |
| E | 0 | HIS | - | EXPRESSION TAG | UNP P53011 |
| F | -1 | PRO | - | EXPRESSION TAG | UNP P53011 |
| F | 0 | HIS | - | EXPRESSION TAG | UNP P53011 |

- Molecule 2 is a protein called Nucleoporin NUP85.

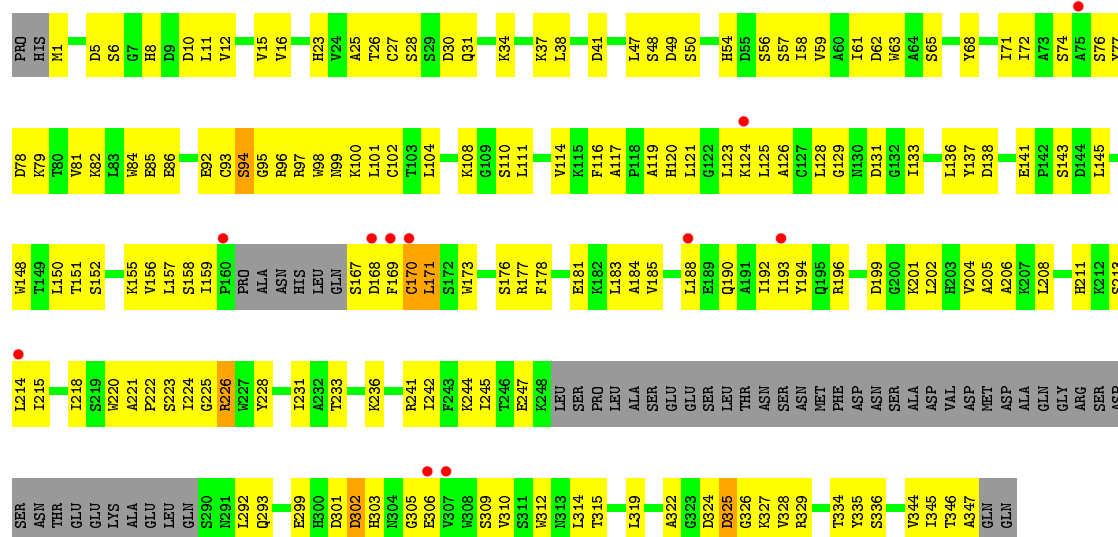
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | C | 492 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3938 | 2526 | 634 | 756 | 22 | | | |
| 2 | D | 480 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3850 | 2473 | 618 | 737 | 22 | | | |
| 2 | G | 482 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3863 | 2482 | 620 | 739 | 22 | | | |
| 2 | H | 493 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3947 | 2532 | 636 | 757 | 22 | | | |

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

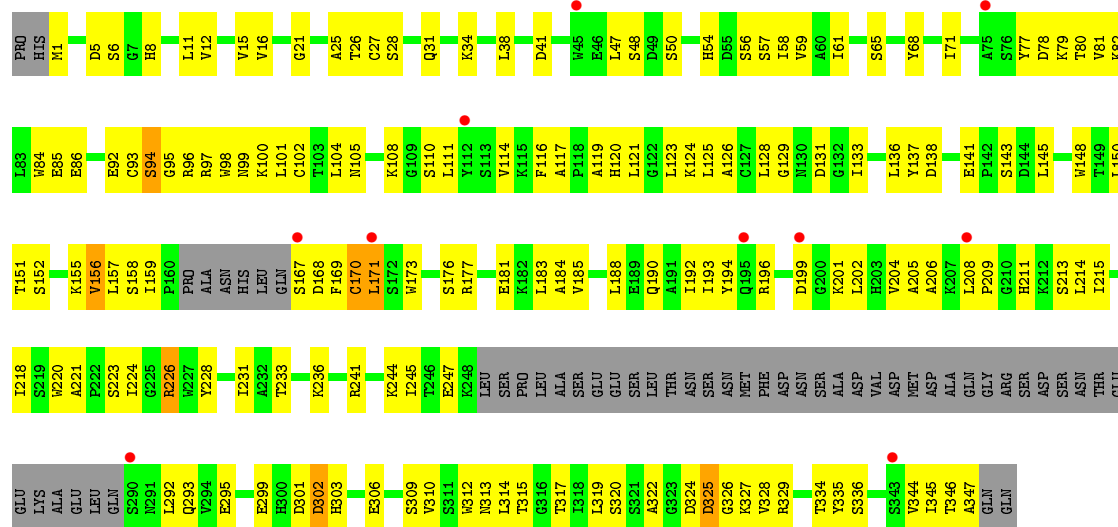
Chain A: 

[illegible]

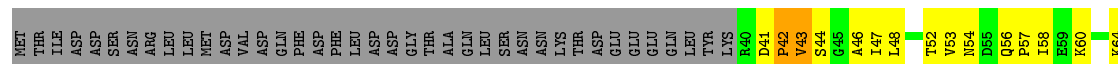
- Molecule 1: Nucleoporin SEH1

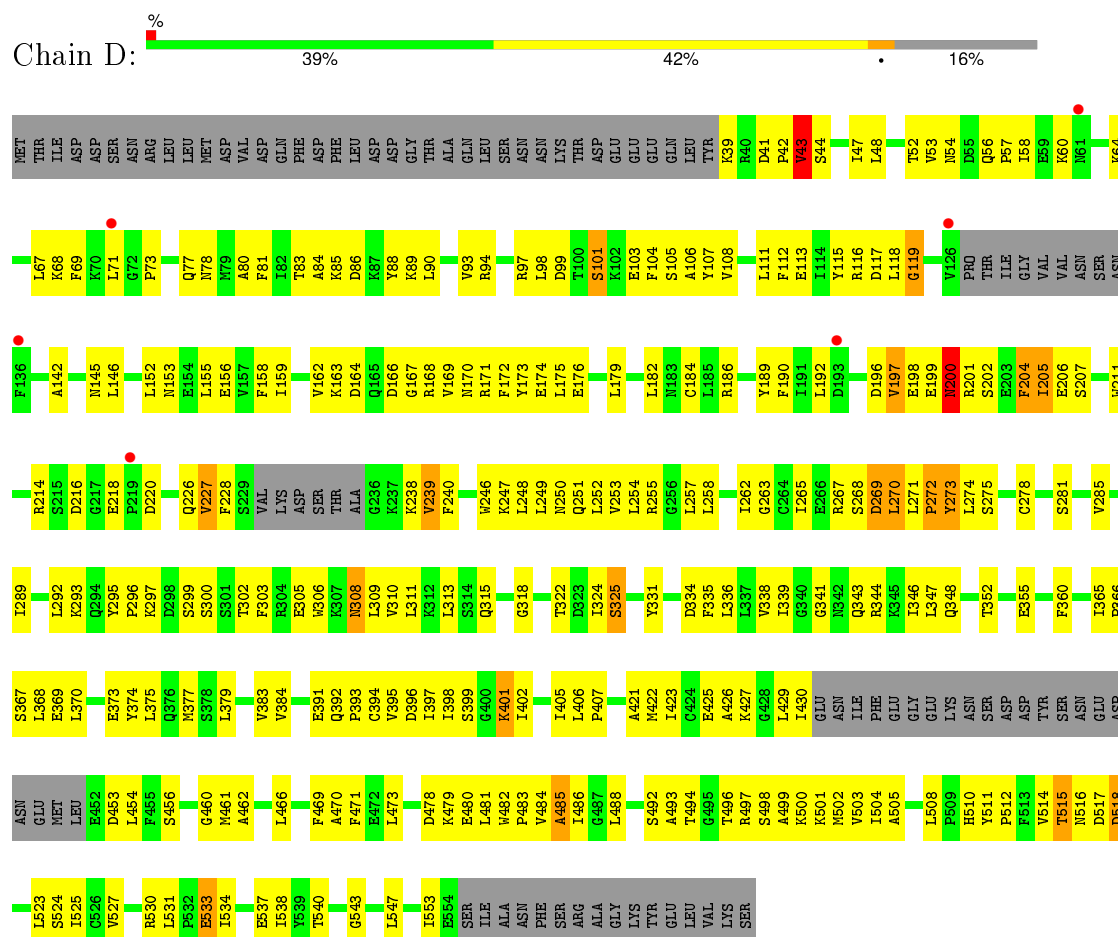


- Molecule 1: Nucleoporin SEH1

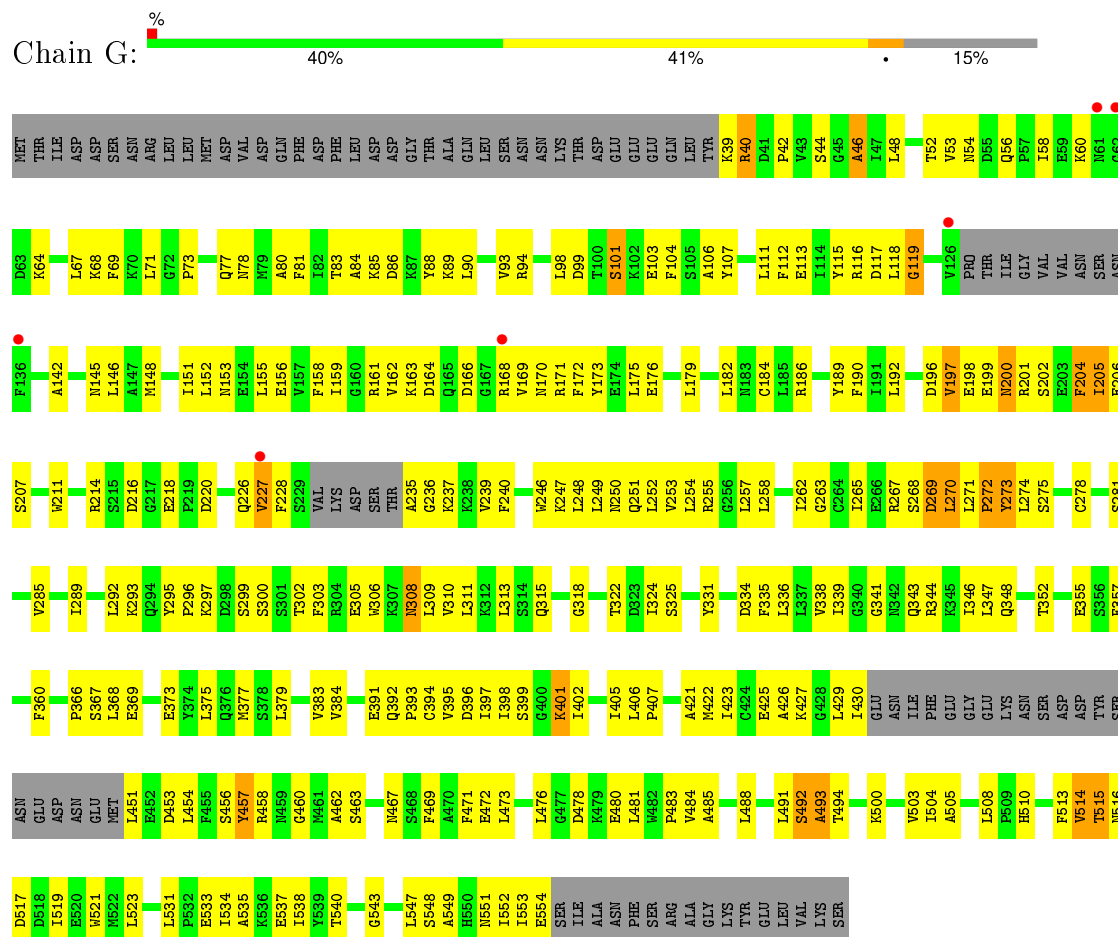


- Molecule 2: Nucleoporin NUP85

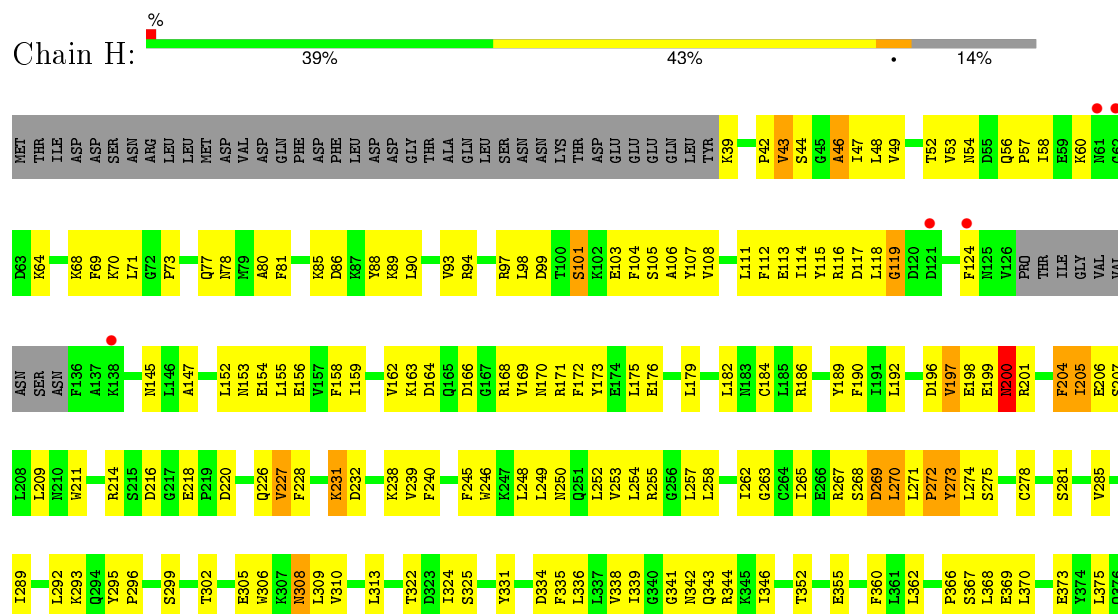


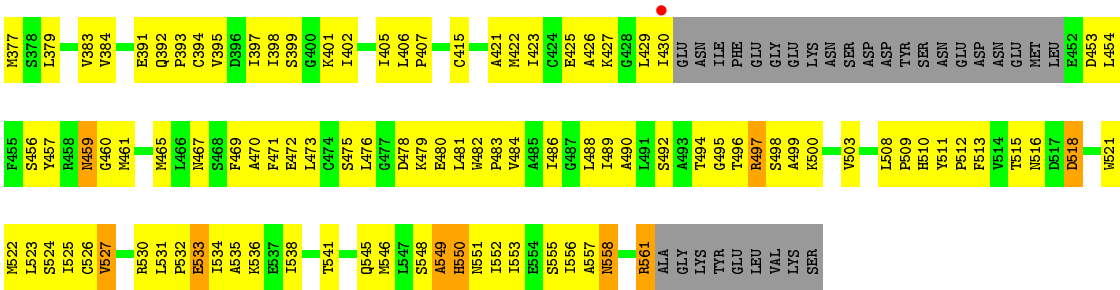


- Molecule 2: Nucleoporin NUP85



- Molecule 2: Nucleoporin NUP85





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 105.38Å 106.49Å 358.64Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 3.75 47.52 – 3.53 | Depositor EDS |
| % Data completeness (in resolution range) | (Not available) (50.00-3.75) 86.4 (47.52-3.53) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.18 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.74 (at 3.57Å) | Xtriage |
| Refinement program | CNS 1.2 | Depositor |
| R, R_{free} | 0.243 , 0.272 0.254 , 0.280 | Depositor DCC |
| R_{free} test set | 1972 reflections (5.04%) | DCC |
| Wilson B-factor (Å ²) | 107.4 | Xtriage |
| Anisotropy | 0.100 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 78.9 | EDS |
| Estimated twinning fraction | 0.337 for k,h,-l | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Outliers | 1 of 46121 reflections (0.002%) | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 25114 | wwPDB-VP |
| Average B, all atoms (Å ²) | 127.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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 | 0.40 | 0/2437 | 0.64 | 0/3301 |
| 1 | B | 0.39 | 0/2437 | 0.63 | 0/3301 |
| 1 | E | 0.39 | 0/2437 | 0.64 | 0/3301 |
| 1 | F | 0.40 | 0/2437 | 0.64 | 0/3301 |
| 2 | C | 0.58 | 2/4018 (0.0%) | 0.67 | 1/5440 (0.0%) |
| 2 | D | 0.53 | 1/3928 (0.0%) | 0.67 | 2/5316 (0.0%) |
| 2 | G | 0.50 | 1/3941 (0.0%) | 0.66 | 1/5334 (0.0%) |
| 2 | H | 0.59 | 3/4027 (0.1%) | 0.67 | 1/5451 (0.0%) |
| All | All | 0.50 | 7/25662 (0.0%) | 0.66 | 5/34745 (0.0%) |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | H | 39 | LYS | CD-CE | 5.48 | 1.65 | 1.51 |
| 2 | G | 39 | LYS | CD-CE | 5.47 | 1.65 | 1.51 |
| 2 | H | 43 | VAL | CB-CG2 | 5.46 | 1.64 | 1.52 |
| 2 | D | 39 | LYS | CD-CE | 5.43 | 1.64 | 1.51 |
| 2 | C | 552 | ILE | CA-CB | 5.22 | 1.66 | 1.54 |
| 2 | C | 554 | GLU | CD-OE1 | 5.08 | 1.31 | 1.25 |
| 2 | H | 561 | ARG | CZ-NH1 | 5.03 | 1.39 | 1.33 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | D | 41 | ASP | CB-CG-OD1 | 5.93 | 123.64 | 118.30 |
| 2 | C | 43 | VAL | CB-CA-C | -5.84 | 100.30 | 111.40 |
| 2 | D | 43 | VAL | N-CA-C | 5.59 | 126.11 | 111.00 |
| 2 | G | 40 | ARG | CB-CA-C | -5.31 | 99.77 | 110.40 |
| 2 | H | 39 | LYS | CD-CE-NZ | 5.21 | 123.68 | 111.70 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 2379 | 0 | 2319 | 165 | 0 |
| 1 | B | 2379 | 0 | 2319 | 165 | 0 |
| 1 | E | 2379 | 0 | 2319 | 170 | 0 |
| 1 | F | 2379 | 0 | 2319 | 167 | 0 |
| 2 | C | 3938 | 0 | 3892 | 274 | 0 |
| 2 | D | 3850 | 0 | 3807 | 257 | 0 |
| 2 | G | 3863 | 0 | 3823 | 251 | 0 |
| 2 | H | 3947 | 0 | 3905 | 279 | 0 |
| All | All | 25114 | 0 | 24703 | 1642 | 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 33.

All (1642) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:43:VAL:HG13 | 2:C:48:LEU:HD22 | 1.27 | 1.10 |
| 2:D:42:PRO:HB3 | 2:D:48:LEU:HD22 | 1.37 | 1.04 |
| 2:H:42:PRO:HB3 | 2:H:48:LEU:HD22 | 1.42 | 0.99 |
| 2:H:42:PRO:HD3 | 2:H:48:LEU:HB2 | 1.40 | 0.99 |
| 2:D:42:PRO:CG | 2:D:48:LEU:HB2 | 1.94 | 0.98 |
| 2:D:515:THR:HG22 | 2:D:517:ASP:H | 1.24 | 0.98 |
| 1:A:211:HIS:NE2 | 1:A:233:THR:HG21 | 1.79 | 0.97 |
| 2:C:43:VAL:CG1 | 2:C:48:LEU:HD22 | 1.94 | 0.97 |
| 1:F:211:HIS:NE2 | 1:F:233:THR:HG21 | 1.81 | 0.95 |
| 1:B:211:HIS:NE2 | 1:B:233:THR:HG21 | 1.84 | 0.93 |
| 2:H:42:PRO:CD | 2:H:48:LEU:HB2 | 1.99 | 0.92 |
| 1:B:81:VAL:HG23 | 1:B:111:LEU:HD13 | 1.49 | 0.92 |
| 1:E:81:VAL:HG23 | 1:E:111:LEU:HD13 | 1.49 | 0.91 |
| 1:F:81:VAL:HG23 | 1:F:111:LEU:HD13 | 1.52 | 0.91 |
| 1:E:211:HIS:NE2 | 1:E:233:THR:HG21 | 1.84 | 0.91 |
| 2:G:42:PRO:HD3 | 2:G:48:LEU:HB2 | 1.51 | 0.91 |
| 1:A:81:VAL:HG23 | 1:A:111:LEU:HD13 | 1.50 | 0.90 |
| 1:B:27:CYS:HB3 | 1:B:61:ILE:HD11 | 1.51 | 0.89 |
| 2:H:231:LYS:HE3 | 2:H:238:LYS:HG2 | 1.53 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:42:PRO:CB | 2:D:48:LEU:HB2 | 2.03 | 0.88 |
| 1:F:220:TRP:HA | 1:F:231:ILE:HG22 | 1.55 | 0.88 |
| 2:G:453:ASP:HB2 | 2:G:456:SER:HB2 | 1.54 | 0.87 |
| 1:E:27:CYS:HB3 | 1:E:61:ILE:HD11 | 1.56 | 0.87 |
| 1:A:220:TRP:HA | 1:A:231:ILE:HG22 | 1.57 | 0.86 |
| 2:D:42:PRO:HB3 | 2:D:48:LEU:HB2 | 1.58 | 0.85 |
| 2:C:515:THR:HG22 | 2:C:517:ASP:H | 1.41 | 0.85 |
| 1:A:27:CYS:HB3 | 1:A:61:ILE:HD11 | 1.59 | 0.84 |
| 2:C:553:ILE:O | 2:C:556:ILE:HB | 1.77 | 0.83 |
| 2:D:515:THR:HG22 | 2:D:517:ASP:N | 1.94 | 0.83 |
| 1:E:220:TRP:HA | 1:E:231:ILE:HG22 | 1.61 | 0.83 |
| 2:G:515:THR:HG22 | 2:G:517:ASP:H | 1.43 | 0.82 |
| 1:F:27:CYS:HB3 | 1:F:61:ILE:HD11 | 1.60 | 0.82 |
| 1:A:213:SER:HB3 | 1:A:236:LYS:HB3 | 1.62 | 0.82 |
| 1:A:12:VAL:HA | 1:A:28:SER:HB3 | 1.61 | 0.81 |
| 2:D:422:MET:HB2 | 2:D:466:LEU:HD11 | 1.62 | 0.81 |
| 2:H:42:PRO:HD3 | 2:H:48:LEU:CB | 2.09 | 0.81 |
| 1:A:11:LEU:O | 1:A:28:SER:HB2 | 1.80 | 0.81 |
| 1:F:104:LEU:HD13 | 1:F:137:TYR:CD2 | 2.16 | 0.81 |
| 1:B:104:LEU:HD13 | 1:B:137:TYR:CD2 | 2.16 | 0.80 |
| 2:H:499:ALA:O | 2:H:503:VAL:HG23 | 1.80 | 0.80 |
| 1:E:104:LEU:HD13 | 1:E:137:TYR:CD2 | 2.15 | 0.80 |
| 2:D:249:LEU:O | 2:D:253:VAL:HG23 | 1.80 | 0.80 |
| 1:B:220:TRP:HA | 1:B:231:ILE:HG22 | 1.63 | 0.80 |
| 2:C:231:LYS:HE3 | 2:C:233:SER:HB3 | 1.64 | 0.80 |
| 1:F:11:LEU:O | 1:F:28:SER:HB2 | 1.82 | 0.80 |
| 1:B:213:SER:HB3 | 1:B:236:LYS:HB3 | 1.64 | 0.80 |
| 1:F:12:VAL:HA | 1:F:28:SER:HB3 | 1.62 | 0.80 |
| 1:E:11:LEU:O | 1:E:28:SER:HB2 | 1.81 | 0.79 |
| 2:D:258:LEU:HD22 | 2:D:292:LEU:HD22 | 1.65 | 0.79 |
| 2:D:480:GLU:O | 2:D:483:PRO:HD2 | 1.83 | 0.79 |
| 1:F:213:SER:HB3 | 1:F:236:LYS:HB3 | 1.65 | 0.79 |
| 1:A:104:LEU:HD13 | 1:A:137:TYR:CD2 | 2.17 | 0.79 |
| 2:D:42:PRO:CD | 2:D:48:LEU:HB2 | 2.13 | 0.78 |
| 1:B:27:CYS:CB | 1:B:61:ILE:HD11 | 2.13 | 0.78 |
| 2:H:515:THR:HG22 | 2:H:516:ASN:H | 1.47 | 0.78 |
| 2:H:521:TRP:CZ2 | 2:H:525:ILE:HD11 | 2.19 | 0.78 |
| 1:E:213:SER:HB3 | 1:E:236:LYS:HB3 | 1.66 | 0.78 |
| 2:G:453:ASP:CB | 2:G:456:SER:HB2 | 2.14 | 0.78 |
| 2:H:47:ILE:CD1 | 2:H:97:ARG:HE | 1.96 | 0.78 |
| 2:D:42:PRO:HB3 | 2:D:48:LEU:CD2 | 2.13 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:249:LEU:O | 2:G:253:VAL:HG23 | 1.83 | 0.78 |
| 2:D:296:PRO:HG3 | 2:D:302:THR:HG22 | 1.66 | 0.77 |
| 2:G:296:PRO:HG3 | 2:G:302:THR:HG22 | 1.65 | 0.77 |
| 2:C:249:LEU:O | 2:C:253:VAL:HG23 | 1.83 | 0.77 |
| 2:C:258:LEU:HD22 | 2:C:292:LEU:HD22 | 1.66 | 0.77 |
| 2:H:553:ILE:CA | 2:H:556:ILE:HG22 | 2.15 | 0.76 |
| 1:A:211:HIS:CD2 | 1:A:233:THR:HG21 | 2.21 | 0.76 |
| 2:G:258:LEU:HD22 | 2:G:292:LEU:HD22 | 1.67 | 0.76 |
| 2:H:69:PHE:HE1 | 2:H:71:LEU:HD23 | 1.50 | 0.75 |
| 1:E:27:CYS:CB | 1:E:61:ILE:HD11 | 2.16 | 0.75 |
| 2:C:478:ASP:OD1 | 2:C:480:GLU:HB2 | 1.85 | 0.75 |
| 2:H:258:LEU:HD22 | 2:H:292:LEU:HD22 | 1.68 | 0.75 |
| 2:H:296:PRO:HG3 | 2:H:302:THR:HG22 | 1.69 | 0.75 |
| 1:F:211:HIS:CD2 | 1:F:233:THR:HG21 | 2.20 | 0.75 |
| 1:B:211:HIS:CD2 | 1:B:233:THR:HG21 | 2.21 | 0.75 |
| 2:C:406:LEU:HB2 | 2:C:407:PRO:HD3 | 1.67 | 0.75 |
| 2:G:42:PRO:CD | 2:G:48:LEU:HB2 | 2.16 | 0.75 |
| 1:E:12:VAL:HA | 1:E:28:SER:HB3 | 1.67 | 0.75 |
| 1:F:54:HIS:HB3 | 1:F:78:ASP:OD2 | 1.86 | 0.75 |
| 2:G:344:ARG:HG3 | 2:G:344:ARG:HH11 | 1.51 | 0.75 |
| 2:H:344:ARG:HG3 | 2:H:344:ARG:HH11 | 1.51 | 0.75 |
| 2:C:296:PRO:HG3 | 2:C:302:THR:HG22 | 1.69 | 0.75 |
| 2:C:69:PHE:HE1 | 2:C:71:LEU:HD23 | 1.51 | 0.75 |
| 2:D:454:LEU:HD23 | 2:D:503:VAL:HG21 | 1.69 | 0.75 |
| 1:B:11:LEU:O | 1:B:28:SER:HB2 | 1.87 | 0.75 |
| 2:H:515:THR:HG22 | 2:H:516:ASN:N | 2.01 | 0.75 |
| 2:D:42:PRO:HD3 | 2:D:48:LEU:N | 2.02 | 0.74 |
| 2:G:278:CYS:HB2 | 2:G:324:ILE:HG23 | 1.68 | 0.74 |
| 1:E:324:ASP:HB3 | 2:G:64:LYS:HG2 | 1.70 | 0.74 |
| 1:A:208:LEU:HD11 | 1:A:231:ILE:CD1 | 2.16 | 0.74 |
| 1:B:54:HIS:HB3 | 1:B:78:ASP:OD2 | 1.88 | 0.74 |
| 1:E:211:HIS:CD2 | 1:E:233:THR:HG21 | 2.22 | 0.74 |
| 2:H:533:GLU:OE1 | 2:H:533:GLU:HA | 1.88 | 0.74 |
| 1:F:208:LEU:HD11 | 1:F:231:ILE:CD1 | 2.18 | 0.74 |
| 1:E:208:LEU:HD11 | 1:E:231:ILE:CD1 | 2.17 | 0.74 |
| 2:C:344:ARG:HG3 | 2:C:344:ARG:HH11 | 1.50 | 0.74 |
| 2:H:454:LEU:HD23 | 2:H:503:VAL:HG21 | 1.70 | 0.74 |
| 2:C:550:HIS:HA | 2:C:553:ILE:CD1 | 2.17 | 0.73 |
| 2:H:406:LEU:HB2 | 2:H:407:PRO:HD3 | 1.69 | 0.73 |
| 2:C:499:ALA:O | 2:C:503:VAL:HG23 | 1.87 | 0.73 |
| 1:F:27:CYS:CB | 1:F:61:ILE:HD11 | 2.18 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:555:SER:HA | 2:C:558:ASN:OD1 | 1.87 | 0.73 |
| 2:D:344:ARG:HG3 | 2:D:344:ARG:HH11 | 1.52 | 0.73 |
| 2:H:249:LEU:O | 2:H:253:VAL:HG23 | 1.87 | 0.73 |
| 1:A:27:CYS:CB | 1:A:61:ILE:HD11 | 2.19 | 0.73 |
| 1:F:324:ASP:HB3 | 2:H:64:LYS:HG2 | 1.71 | 0.73 |
| 2:D:406:LEU:HB2 | 2:D:407:PRO:HD3 | 1.71 | 0.72 |
| 2:D:69:PHE:HE1 | 2:D:71:LEU:HD23 | 1.52 | 0.72 |
| 1:A:54:HIS:HB3 | 1:A:78:ASP:OD2 | 1.89 | 0.72 |
| 2:G:480:GLU:O | 2:G:483:PRO:HD2 | 1.89 | 0.72 |
| 1:B:12:VAL:HA | 1:B:28:SER:HB3 | 1.69 | 0.72 |
| 1:E:54:HIS:HB3 | 1:E:78:ASP:OD2 | 1.88 | 0.72 |
| 2:H:42:PRO:CG | 2:H:48:LEU:HB2 | 2.18 | 0.72 |
| 1:B:81:VAL:HG23 | 1:B:111:LEU:CD1 | 2.19 | 0.72 |
| 2:G:335:PHE:O | 2:G:339:ILE:HG13 | 1.89 | 0.72 |
| 2:G:69:PHE:HE1 | 2:G:71:LEU:HD23 | 1.55 | 0.72 |
| 2:H:184:CYS:HB2 | 2:H:211:TRP:NE1 | 2.05 | 0.72 |
| 2:H:478:ASP:OD1 | 2:H:480:GLU:HB2 | 1.89 | 0.72 |
| 2:H:278:CYS:HB2 | 2:H:324:ILE:HG23 | 1.71 | 0.72 |
| 1:F:124:LYS:HG3 | 1:F:138:ASP:HB3 | 1.72 | 0.71 |
| 2:G:406:LEU:HB2 | 2:G:407:PRO:HD3 | 1.72 | 0.71 |
| 1:B:208:LEU:HD11 | 1:B:231:ILE:CD1 | 2.20 | 0.71 |
| 2:H:552:ILE:O | 2:H:556:ILE:N | 2.23 | 0.71 |
| 2:H:335:PHE:O | 2:H:339:ILE:HG13 | 1.90 | 0.71 |
| 1:F:334:THR:HG22 | 1:F:335:TYR:N | 2.05 | 0.71 |
| 2:H:511:TYR:HD2 | 2:H:522:MET:SD | 2.13 | 0.71 |
| 2:D:184:CYS:HB2 | 2:D:211:TRP:NE1 | 2.05 | 0.71 |
| 2:G:402:ILE:HD12 | 2:G:429:LEU:HB3 | 1.71 | 0.71 |
| 2:D:278:CYS:HB2 | 2:D:324:ILE:HG23 | 1.71 | 0.71 |
| 2:D:43:VAL:HG23 | 2:D:44:SER:H | 1.56 | 0.71 |
| 2:C:402:ILE:HD12 | 2:C:429:LEU:HB3 | 1.71 | 0.71 |
| 2:C:278:CYS:HB2 | 2:C:324:ILE:HG23 | 1.72 | 0.71 |
| 1:E:334:THR:HG22 | 1:E:335:TYR:N | 2.05 | 0.71 |
| 2:C:454:LEU:HD23 | 2:C:503:VAL:HG21 | 1.73 | 0.71 |
| 2:H:484:VAL:O | 2:H:488:LEU:HB2 | 1.91 | 0.70 |
| 1:B:324:ASP:HB3 | 2:D:64:LYS:HG2 | 1.73 | 0.70 |
| 2:D:402:ILE:HD12 | 2:D:429:LEU:HB3 | 1.73 | 0.70 |
| 2:C:550:HIS:HA | 2:C:553:ILE:HD12 | 1.72 | 0.70 |
| 2:G:523:LEU:HD21 | 2:G:538:ILE:HG21 | 1.73 | 0.70 |
| 1:B:334:THR:HG22 | 1:B:335:TYR:N | 2.05 | 0.70 |
| 1:A:124:LYS:HG3 | 1:A:138:ASP:HB3 | 1.74 | 0.70 |
| 2:C:335:PHE:O | 2:C:339:ILE:HG13 | 1.91 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:326:GLY:HA3 | 2:H:58:ILE:HD12 | 1.73 | 0.70 |
| 1:E:81:VAL:HG23 | 1:E:111:LEU:CD1 | 2.21 | 0.70 |
| 1:F:214:LEU:HD12 | 1:F:214:LEU:H | 1.57 | 0.70 |
| 2:D:335:PHE:O | 2:D:339:ILE:HG13 | 1.91 | 0.69 |
| 2:G:515:THR:HG22 | 2:G:516:ASN:N | 2.05 | 0.69 |
| 1:A:334:THR:HG22 | 1:A:335:TYR:N | 2.06 | 0.69 |
| 1:F:345:ILE:HD13 | 2:H:93:VAL:HG11 | 1.74 | 0.69 |
| 2:G:98:LEU:HD11 | 2:G:476:LEU:HD11 | 1.73 | 0.69 |
| 2:G:454:LEU:HD23 | 2:G:503:VAL:HG21 | 1.74 | 0.69 |
| 2:H:402:ILE:HD12 | 2:H:429:LEU:HB3 | 1.74 | 0.69 |
| 2:H:553:ILE:C | 2:H:556:ILE:HG22 | 2.13 | 0.69 |
| 2:H:555:SER:HA | 2:H:558:ASN:HB3 | 1.73 | 0.69 |
| 2:H:553:ILE:HA | 2:H:556:ILE:CG2 | 2.22 | 0.69 |
| 2:C:252:LEU:HD23 | 2:C:257:LEU:HD12 | 1.73 | 0.69 |
| 2:H:252:LEU:HD23 | 2:H:257:LEU:HD12 | 1.74 | 0.69 |
| 1:F:27:CYS:SG | 1:F:61:ILE:HD11 | 2.34 | 0.68 |
| 2:G:184:CYS:HB2 | 2:G:211:TRP:NE1 | 2.08 | 0.68 |
| 2:C:184:CYS:HB2 | 2:C:211:TRP:NE1 | 2.08 | 0.68 |
| 2:C:196:ASP:O | 2:C:198:GLU:N | 2.27 | 0.68 |
| 2:H:231:LYS:HG3 | 2:H:232:ASP:H | 1.57 | 0.68 |
| 1:A:324:ASP:HB3 | 2:C:64:LYS:HG2 | 1.75 | 0.68 |
| 2:G:196:ASP:O | 2:G:198:GLU:N | 2.26 | 0.68 |
| 2:H:68:LYS:HB2 | 2:H:81:PHE:CE1 | 2.28 | 0.68 |
| 2:G:531:LEU:HD13 | 2:G:534:ILE:HD12 | 1.75 | 0.68 |
| 2:H:548:SER:O | 2:H:552:ILE:HG13 | 1.94 | 0.68 |
| 2:C:515:THR:HG22 | 2:C:516:ASN:N | 2.09 | 0.68 |
| 1:F:236:LYS:O | 1:F:306:GLU:HG2 | 1.94 | 0.68 |
| 2:C:265:ILE:HG21 | 2:C:289:ILE:HD11 | 1.76 | 0.68 |
| 2:C:68:LYS:HB2 | 2:C:81:PHE:CE1 | 2.29 | 0.68 |
| 1:A:81:VAL:HG23 | 1:A:111:LEU:CD1 | 2.22 | 0.67 |
| 2:C:227:VAL:HG21 | 2:C:248:LEU:HD12 | 1.75 | 0.67 |
| 2:H:196:ASP:O | 2:H:198:GLU:N | 2.27 | 0.67 |
| 1:A:71:ILE:HD11 | 1:A:145:LEU:HD23 | 1.76 | 0.67 |
| 2:G:265:ILE:HG21 | 2:G:289:ILE:HD11 | 1.76 | 0.67 |
| 2:D:341:GLY:HA2 | 2:D:346:ILE:HD11 | 1.76 | 0.67 |
| 1:A:236:LYS:O | 1:A:306:GLU:HG2 | 1.95 | 0.67 |
| 2:G:278:CYS:CB | 2:G:324:ILE:HG23 | 2.24 | 0.67 |
| 2:G:252:LEU:HD23 | 2:G:257:LEU:HD12 | 1.76 | 0.67 |
| 1:A:167:SER:HA | 1:A:188:LEU:CD2 | 2.25 | 0.67 |
| 1:F:11:LEU:HD12 | 1:F:11:LEU:O | 1.94 | 0.67 |
| 1:A:177:ARG:O | 1:A:177:ARG:HG2 | 1.95 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:71:ILE:HD11 | 1:F:145:LEU:HD23 | 1.77 | 0.67 |
| 1:B:85:GLU:HB3 | 1:B:101:LEU:HD21 | 1.77 | 0.67 |
| 2:H:47:ILE:HD13 | 2:H:97:ARG:HE | 1.60 | 0.67 |
| 1:F:167:SER:HA | 1:F:188:LEU:CD2 | 2.24 | 0.67 |
| 2:C:89:LYS:N | 2:C:89:LYS:HD2 | 2.09 | 0.67 |
| 1:E:236:LYS:O | 1:E:306:GLU:HG2 | 1.94 | 0.67 |
| 2:C:118:LEU:HD21 | 2:C:147:ALA:HB2 | 1.77 | 0.67 |
| 1:A:65:SER:OG | 1:A:119:ALA:HB2 | 1.95 | 0.67 |
| 2:D:89:LYS:HD2 | 2:D:89:LYS:N | 2.09 | 0.66 |
| 1:B:124:LYS:HG3 | 1:B:138:ASP:HB3 | 1.77 | 0.66 |
| 2:H:541:THR:O | 2:H:545:GLN:HG3 | 1.95 | 0.66 |
| 2:G:89:LYS:N | 2:G:89:LYS:HD2 | 2.10 | 0.66 |
| 2:G:169:VAL:HG12 | 2:G:170:ASN:H | 1.59 | 0.66 |
| 1:F:85:GLU:HB3 | 1:F:101:LEU:HD21 | 1.78 | 0.66 |
| 2:C:511:TYR:HD2 | 2:C:522:MET:SD | 2.19 | 0.66 |
| 2:C:533:GLU:OE1 | 2:C:536:LYS:HD2 | 1.96 | 0.66 |
| 1:A:214:LEU:HD12 | 1:A:214:LEU:H | 1.60 | 0.66 |
| 1:A:209:PRO:HG3 | 2:D:315:GLN:HA | 1.77 | 0.66 |
| 1:B:214:LEU:H | 1:B:214:LEU:HD12 | 1.61 | 0.66 |
| 2:H:89:LYS:HD2 | 2:H:89:LYS:N | 2.11 | 0.66 |
| 2:H:240:PHE:CE2 | 2:H:269:ASP:HB3 | 2.31 | 0.66 |
| 2:D:196:ASP:O | 2:D:198:GLU:N | 2.29 | 0.66 |
| 2:G:341:GLY:HA2 | 2:G:346:ILE:HD11 | 1.77 | 0.66 |
| 2:D:42:PRO:HD3 | 2:D:48:LEU:HB2 | 1.75 | 0.66 |
| 1:E:241:ARG:HH11 | 1:E:241:ARG:HG2 | 1.60 | 0.66 |
| 1:E:27:CYS:SG | 1:E:61:ILE:HD11 | 2.35 | 0.66 |
| 1:B:11:LEU:HD12 | 1:B:11:LEU:O | 1.96 | 0.66 |
| 2:H:105:SER:HB2 | 2:H:481:LEU:HD21 | 1.77 | 0.66 |
| 1:E:214:LEU:HD12 | 1:E:214:LEU:H | 1.60 | 0.66 |
| 2:H:454:LEU:HB2 | 2:H:499:ALA:HB1 | 1.78 | 0.66 |
| 2:D:42:PRO:HB3 | 2:D:48:LEU:CB | 2.26 | 0.66 |
| 1:E:167:SER:HA | 1:E:188:LEU:CD2 | 2.26 | 0.66 |
| 2:C:41:ASP:O | 2:C:48:LEU:N | 2.27 | 0.65 |
| 1:B:236:LYS:O | 1:B:306:GLU:HG2 | 1.96 | 0.65 |
| 1:B:329:ARG:HG2 | 1:B:344:VAL:HG22 | 1.77 | 0.65 |
| 2:D:201:ARG:CZ | 2:D:205:ILE:HD11 | 2.26 | 0.65 |
| 1:E:329:ARG:HH12 | 2:G:44:SER:HB2 | 1.62 | 0.65 |
| 1:B:177:ARG:O | 1:B:177:ARG:HG2 | 1.96 | 0.65 |
| 2:G:42:PRO:HB3 | 2:G:48:LEU:HD22 | 1.79 | 0.65 |
| 1:A:326:GLY:HA3 | 2:C:58:ILE:HD12 | 1.78 | 0.65 |
| 2:D:523:LEU:HD21 | 2:D:538:ILE:HG21 | 1.77 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:42:PRO:HG3 | 2:D:48:LEU:HB2 | 1.77 | 0.65 |
| 1:F:81:VAL:HG23 | 1:F:111:LEU:CD1 | 2.25 | 0.65 |
| 2:H:265:ILE:HG21 | 2:H:289:ILE:HD11 | 1.78 | 0.65 |
| 1:F:177:ARG:O | 1:F:177:ARG:HG2 | 1.95 | 0.65 |
| 1:B:159:ILE:HG22 | 1:B:159:ILE:O | 1.97 | 0.65 |
| 1:E:124:LYS:HG3 | 1:E:138:ASP:HB3 | 1.77 | 0.65 |
| 2:H:255:ARG:HB2 | 2:H:257:LEU:HG | 1.77 | 0.65 |
| 2:C:418:ALA:HB1 | 2:C:466:LEU:HD23 | 1.78 | 0.65 |
| 2:H:533:GLU:OE1 | 2:H:536:LYS:HD2 | 1.96 | 0.65 |
| 2:C:124:PHE:HB2 | 2:C:426:ALA:O | 1.97 | 0.65 |
| 1:E:159:ILE:HG22 | 1:E:159:ILE:O | 1.97 | 0.65 |
| 1:A:345:ILE:HD13 | 2:C:93:VAL:HG11 | 1.79 | 0.65 |
| 1:E:177:ARG:HG2 | 1:E:177:ARG:O | 1.97 | 0.65 |
| 1:B:27:CYS:SG | 1:B:61:ILE:HD11 | 2.37 | 0.65 |
| 1:A:27:CYS:SG | 1:A:61:ILE:HD11 | 2.37 | 0.64 |
| 2:H:335:PHE:CE2 | 2:H:339:ILE:HD11 | 2.32 | 0.64 |
| 2:H:278:CYS:CB | 2:H:324:ILE:HG23 | 2.27 | 0.64 |
| 2:D:278:CYS:CB | 2:D:324:ILE:HG23 | 2.27 | 0.64 |
| 2:H:546:MET:O | 2:H:549:ALA:HB3 | 1.98 | 0.64 |
| 2:C:255:ARG:HB2 | 2:C:257:LEU:HG | 1.78 | 0.64 |
| 2:C:480:GLU:O | 2:C:483:PRO:HD2 | 1.97 | 0.64 |
| 2:C:278:CYS:HB3 | 2:C:281:SER:HB2 | 1.79 | 0.64 |
| 1:F:329:ARG:HG2 | 1:F:344:VAL:HG22 | 1.78 | 0.64 |
| 1:B:241:ARG:HG2 | 1:B:241:ARG:HH11 | 1.62 | 0.64 |
| 2:C:201:ARG:CZ | 2:C:205:ILE:HD11 | 2.27 | 0.64 |
| 2:G:240:PHE:CE2 | 2:G:269:ASP:HB3 | 2.32 | 0.64 |
| 1:B:71:ILE:HD11 | 1:B:145:LEU:HD23 | 1.79 | 0.64 |
| 2:D:240:PHE:CE2 | 2:D:269:ASP:HB3 | 2.32 | 0.64 |
| 1:A:241:ARG:HG2 | 1:A:241:ARG:HH11 | 1.61 | 0.64 |
| 1:A:85:GLU:HB3 | 1:A:101:LEU:HD21 | 1.80 | 0.64 |
| 2:C:335:PHE:CE2 | 2:C:339:ILE:HD11 | 2.32 | 0.64 |
| 2:D:169:VAL:HG12 | 2:D:170:ASN:H | 1.62 | 0.64 |
| 1:E:208:LEU:HD11 | 1:E:231:ILE:HD11 | 1.80 | 0.64 |
| 1:F:167:SER:HA | 1:F:188:LEU:HD21 | 1.80 | 0.64 |
| 1:E:205:ALA:HB1 | 1:E:292:LEU:HD12 | 1.79 | 0.64 |
| 2:D:252:LEU:HD23 | 2:D:257:LEU:HD12 | 1.78 | 0.64 |
| 2:G:201:ARG:CZ | 2:G:205:ILE:HD11 | 2.28 | 0.64 |
| 2:H:278:CYS:HB3 | 2:H:281:SER:HB2 | 1.80 | 0.64 |
| 2:C:169:VAL:HG12 | 2:C:170:ASN:H | 1.62 | 0.64 |
| 2:C:240:PHE:CE2 | 2:C:269:ASP:HB3 | 2.33 | 0.63 |
| 2:H:201:ARG:CZ | 2:H:205:ILE:HD11 | 2.28 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:11:LEU:O | 1:A:11:LEU:HD12 | 1.98 | 0.63 |
| 2:C:114:ILE:HD11 | 2:C:154:GLU:HG3 | 1.81 | 0.63 |
| 2:H:118:LEU:HD21 | 2:H:147:ALA:HB2 | 1.80 | 0.63 |
| 1:F:159:ILE:O | 1:F:159:ILE:HG22 | 1.97 | 0.63 |
| 1:A:167:SER:HA | 1:A:188:LEU:HD21 | 1.81 | 0.63 |
| 1:F:65:SER:OG | 1:F:119:ALA:HB2 | 1.98 | 0.63 |
| 1:A:12:VAL:HA | 1:A:28:SER:CB | 2.29 | 0.63 |
| 2:C:278:CYS:CB | 2:C:324:ILE:HG23 | 2.28 | 0.63 |
| 1:A:159:ILE:O | 1:A:159:ILE:HG22 | 1.99 | 0.63 |
| 2:G:402:ILE:CD1 | 2:G:429:LEU:HD13 | 2.29 | 0.63 |
| 2:H:169:VAL:HG12 | 2:H:170:ASN:H | 1.64 | 0.63 |
| 1:E:85:GLU:HB3 | 1:E:101:LEU:HD21 | 1.79 | 0.63 |
| 1:E:11:LEU:HD12 | 1:E:11:LEU:O | 1.98 | 0.63 |
| 1:E:329:ARG:HG2 | 1:E:344:VAL:HG22 | 1.80 | 0.63 |
| 2:D:68:LYS:HB2 | 2:D:81:PHE:CE1 | 2.34 | 0.63 |
| 1:F:301:ASP:O | 1:F:303:HIS:N | 2.32 | 0.63 |
| 1:F:335:TYR:HB3 | 2:G:373:GLU:HG3 | 1.80 | 0.63 |
| 2:D:265:ILE:HG21 | 2:D:289:ILE:HD11 | 1.80 | 0.63 |
| 2:H:192:LEU:HD11 | 2:H:204:PHE:CD2 | 2.33 | 0.63 |
| 2:C:546:MET:O | 2:C:549:ALA:HB3 | 1.99 | 0.63 |
| 2:C:43:VAL:HG13 | 2:C:48:LEU:CD2 | 2.18 | 0.63 |
| 1:F:334:THR:HG22 | 1:F:336:SER:H | 1.63 | 0.63 |
| 1:F:241:ARG:HH11 | 1:F:241:ARG:HG2 | 1.63 | 0.63 |
| 2:G:278:CYS:HB3 | 2:G:281:SER:HB2 | 1.80 | 0.62 |
| 2:H:114:ILE:HD11 | 2:H:154:GLU:HG3 | 1.81 | 0.62 |
| 2:G:543:GLY:O | 2:G:547:LEU:HG | 1.99 | 0.62 |
| 2:H:453:ASP:HB3 | 2:H:456:SER:HB2 | 1.81 | 0.62 |
| 2:D:531:LEU:HD13 | 2:D:534:ILE:HD12 | 1.81 | 0.62 |
| 2:C:192:LEU:HD11 | 2:C:204:PHE:CD2 | 2.35 | 0.62 |
| 2:D:335:PHE:CE2 | 2:D:339:ILE:HD11 | 2.33 | 0.62 |
| 2:G:240:PHE:CD2 | 2:G:268:SER:HB2 | 2.34 | 0.62 |
| 1:E:71:ILE:HD11 | 1:E:145:LEU:HD23 | 1.80 | 0.62 |
| 2:H:531:LEU:HD13 | 2:H:534:ILE:HD12 | 1.80 | 0.62 |
| 2:G:197:VAL:O | 2:G:197:VAL:HG12 | 1.99 | 0.62 |
| 2:C:496:THR:HG22 | 2:C:497:ARG:H | 1.65 | 0.62 |
| 2:H:341:GLY:HA2 | 2:H:346:ILE:HD11 | 1.82 | 0.62 |
| 2:H:480:GLU:O | 2:H:483:PRO:HD2 | 1.98 | 0.62 |
| 1:A:334:THR:HG22 | 1:A:336:SER:H | 1.65 | 0.62 |
| 2:G:68:LYS:HB2 | 2:G:81:PHE:CE1 | 2.34 | 0.62 |
| 1:E:65:SER:OG | 1:E:119:ALA:HB2 | 2.00 | 0.62 |
| 2:D:42:PRO:HD3 | 2:D:48:LEU:CB | 2.29 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:208:LEU:HD11 | 1:A:231:ILE:HD11 | 1.80 | 0.62 |
| 2:C:541:THR:O | 2:C:545:GLN:HG3 | 2.00 | 0.62 |
| 1:B:31:GLN:HG2 | 1:B:56:SER:O | 2.00 | 0.62 |
| 1:A:329:ARG:HH12 | 2:C:44:SER:HB2 | 1.64 | 0.61 |
| 2:D:255:ARG:HB2 | 2:D:257:LEU:HG | 1.81 | 0.61 |
| 1:F:12:VAL:HA | 1:F:28:SER:CB | 2.30 | 0.61 |
| 2:D:278:CYS:HB3 | 2:D:281:SER:HB2 | 1.81 | 0.61 |
| 2:D:402:ILE:CD1 | 2:D:429:LEU:HD13 | 2.30 | 0.61 |
| 2:H:197:VAL:O | 2:H:197:VAL:HG12 | 1.99 | 0.61 |
| 2:C:197:VAL:HG12 | 2:C:197:VAL:O | 1.99 | 0.61 |
| 2:D:240:PHE:CD2 | 2:D:269:ASP:HB3 | 2.35 | 0.61 |
| 2:G:255:ARG:HB2 | 2:G:257:LEU:HG | 1.80 | 0.61 |
| 2:D:197:VAL:O | 2:D:197:VAL:HG12 | 2.00 | 0.61 |
| 1:B:167:SER:HA | 1:B:188:LEU:CD2 | 2.30 | 0.61 |
| 2:G:552:ILE:C | 2:G:554:GLU:H | 2.04 | 0.61 |
| 1:B:345:ILE:HD13 | 2:D:93:VAL:HG11 | 1.83 | 0.61 |
| 2:H:515:THR:HB | 2:H:518:ASP:OD1 | 2.00 | 0.61 |
| 1:B:159:ILE:HD12 | 1:B:159:ILE:N | 2.15 | 0.61 |
| 1:B:208:LEU:HD11 | 1:B:231:ILE:HD11 | 1.82 | 0.61 |
| 1:F:168:ASP:H | 1:F:188:LEU:HD23 | 1.64 | 0.61 |
| 2:C:240:PHE:CD2 | 2:C:268:SER:HB2 | 2.35 | 0.61 |
| 1:E:168:ASP:H | 1:E:188:LEU:HD23 | 1.65 | 0.61 |
| 2:H:456:SER:OG | 2:H:457:TYR:N | 2.33 | 0.61 |
| 1:B:205:ALA:HB1 | 1:B:292:LEU:HD12 | 1.83 | 0.61 |
| 1:B:131:ASP:OD2 | 1:B:133:ILE:HD12 | 2.01 | 0.61 |
| 2:G:478:ASP:OD1 | 2:G:480:GLU:HB2 | 2.01 | 0.61 |
| 2:H:240:PHE:CD2 | 2:H:268:SER:HB2 | 2.35 | 0.61 |
| 2:C:523:LEU:O | 2:C:526:CYS:HB2 | 2.00 | 0.61 |
| 2:G:107:TYR:CZ | 2:G:111:LEU:HD11 | 2.36 | 0.61 |
| 1:A:329:ARG:HG2 | 1:A:344:VAL:HG22 | 1.81 | 0.60 |
| 1:A:301:ASP:O | 1:A:303:HIS:N | 2.34 | 0.60 |
| 1:E:226:ARG:HH11 | 1:E:226:ARG:HG3 | 1.64 | 0.60 |
| 1:F:214:LEU:HD12 | 1:F:214:LEU:N | 2.16 | 0.60 |
| 2:C:554:GLU:O | 2:C:558:ASN:HB3 | 2.01 | 0.60 |
| 1:A:168:ASP:H | 1:A:188:LEU:HD23 | 1.65 | 0.60 |
| 2:H:334:ASP:O | 2:H:338:VAL:HG23 | 2.01 | 0.60 |
| 1:A:131:ASP:OD2 | 1:A:133:ILE:HD12 | 2.02 | 0.60 |
| 1:E:345:ILE:HD13 | 2:G:93:VAL:HG11 | 1.82 | 0.60 |
| 2:H:553:ILE:O | 2:H:556:ILE:HG22 | 2.02 | 0.60 |
| 1:B:65:SER:OG | 1:B:119:ALA:HB2 | 2.01 | 0.60 |
| 2:C:551:ASN:O | 2:C:554:GLU:HB3 | 2.02 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:302:ASP:OD2 | 2:G:44:SER:HB3 | 2.01 | 0.60 |
| 2:C:459:ASN:OD1 | 2:C:494:THR:HB | 2.00 | 0.60 |
| 2:C:515:THR:CG2 | 2:C:516:ASN:N | 2.65 | 0.60 |
| 2:G:299:SER:HB3 | 2:G:302:THR:OG1 | 2.01 | 0.60 |
| 1:F:183:LEU:HD12 | 1:F:184:ALA:N | 2.16 | 0.60 |
| 2:H:510:HIS:O | 2:H:512:PRO:HD3 | 2.02 | 0.60 |
| 2:H:392:GLN:HB3 | 2:H:393:PRO:HD3 | 1.84 | 0.60 |
| 1:A:312:TRP:CE2 | 1:A:319:LEU:HD13 | 2.36 | 0.60 |
| 2:H:553:ILE:HA | 2:H:556:ILE:HG22 | 1.81 | 0.60 |
| 2:H:240:PHE:CD2 | 2:H:269:ASP:HB3 | 2.37 | 0.60 |
| 2:D:240:PHE:CD2 | 2:D:268:SER:HB2 | 2.36 | 0.60 |
| 1:E:334:THR:HG22 | 1:E:336:SER:H | 1.67 | 0.60 |
| 2:C:341:GLY:HA2 | 2:C:346:ILE:HD11 | 1.84 | 0.60 |
| 1:F:208:LEU:HD11 | 1:F:231:ILE:HD11 | 1.82 | 0.60 |
| 2:D:405:ILE:HG13 | 2:D:406:LEU:N | 2.17 | 0.60 |
| 1:B:334:THR:HG22 | 1:B:336:SER:H | 1.66 | 0.60 |
| 2:D:299:SER:HB3 | 2:D:302:THR:OG1 | 2.01 | 0.59 |
| 1:B:145:LEU:H | 1:B:145:LEU:HD12 | 1.67 | 0.59 |
| 1:A:117:ALA:HB2 | 1:A:173:TRP:CZ2 | 2.37 | 0.59 |
| 1:E:231:ILE:CD1 | 1:E:245:ILE:HD11 | 2.32 | 0.59 |
| 2:G:240:PHE:CD2 | 2:G:269:ASP:HB3 | 2.37 | 0.59 |
| 1:E:131:ASP:OD2 | 1:E:133:ILE:HD12 | 2.02 | 0.59 |
| 1:B:226:ARG:HG3 | 1:B:226:ARG:HH11 | 1.66 | 0.59 |
| 1:E:159:ILE:N | 1:E:159:ILE:HD12 | 2.17 | 0.59 |
| 1:F:312:TRP:CE2 | 1:F:319:LEU:HD13 | 2.36 | 0.59 |
| 1:E:12:VAL:HA | 1:E:28:SER:CB | 2.32 | 0.59 |
| 1:E:117:ALA:HB2 | 1:E:173:TRP:CZ2 | 2.37 | 0.59 |
| 2:G:335:PHE:CE2 | 2:G:339:ILE:HD11 | 2.38 | 0.59 |
| 1:E:225:GLY:HA2 | 2:G:503:VAL:HG22 | 1.85 | 0.59 |
| 2:G:383:VAL:HG12 | 2:G:384:VAL:N | 2.17 | 0.59 |
| 2:H:108:VAL:HG22 | 2:H:469:PHE:HZ | 1.67 | 0.59 |
| 2:C:107:TYR:CZ | 2:C:111:LEU:HD11 | 2.38 | 0.59 |
| 2:C:482:TRP:NE1 | 2:C:512:PRO:HD2 | 2.17 | 0.59 |
| 1:E:84:TRP:HA | 1:E:99:ASN:O | 2.03 | 0.59 |
| 1:A:31:GLN:HG2 | 1:A:56:SER:O | 2.02 | 0.59 |
| 2:G:515:THR:CG2 | 2:G:516:ASN:N | 2.65 | 0.59 |
| 1:E:10:ASP:C | 2:G:88:TYR:HE2 | 2.06 | 0.59 |
| 2:C:392:GLN:HB3 | 2:C:393:PRO:HD3 | 1.85 | 0.59 |
| 1:F:111:LEU:HA | 1:F:129:GLY:HA2 | 1.85 | 0.59 |
| 2:C:240:PHE:CD2 | 2:C:269:ASP:HB3 | 2.38 | 0.59 |
| 2:G:192:LEU:HD11 | 2:G:204:PHE:CD2 | 2.37 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:159:ILE:HD12 | 1:F:159:ILE:N | 2.18 | 0.59 |
| 1:B:301:ASP:O | 1:B:303:HIS:N | 2.36 | 0.59 |
| 2:D:392:GLN:HB3 | 2:D:393:PRO:HD3 | 1.84 | 0.59 |
| 1:F:226:ARG:HG3 | 1:F:226:ARG:HH11 | 1.68 | 0.59 |
| 1:E:167:SER:HA | 1:E:188:LEU:HD21 | 1.84 | 0.59 |
| 2:D:192:LEU:HD11 | 2:D:204:PHE:CD2 | 2.38 | 0.59 |
| 2:C:78:ASN:HB2 | 2:C:93:VAL:O | 2.03 | 0.59 |
| 2:D:383:VAL:HG12 | 2:D:384:VAL:N | 2.18 | 0.59 |
| 1:B:117:ALA:HB2 | 1:B:173:TRP:CZ2 | 2.38 | 0.59 |
| 2:C:231:LYS:CE | 2:C:233:SER:HB3 | 2.30 | 0.58 |
| 1:B:85:GLU:CB | 1:B:101:LEU:HD21 | 2.32 | 0.58 |
| 1:A:159:ILE:N | 1:A:159:ILE:HD12 | 2.18 | 0.58 |
| 1:E:77:TYR:HD1 | 1:E:110:SER:HB2 | 1.67 | 0.58 |
| 2:C:299:SER:HB3 | 2:C:302:THR:OG1 | 2.03 | 0.58 |
| 2:G:274:LEU:HD22 | 2:G:281:SER:HB3 | 1.85 | 0.58 |
| 2:C:383:VAL:HG12 | 2:C:384:VAL:N | 2.18 | 0.58 |
| 2:D:107:TYR:CZ | 2:D:111:LEU:HD11 | 2.38 | 0.58 |
| 2:G:392:GLN:HB3 | 2:G:393:PRO:HD3 | 1.84 | 0.58 |
| 1:E:170:CYS:SG | 1:E:218:ILE:HG22 | 2.42 | 0.58 |
| 2:D:306:TRP:O | 2:D:310:VAL:HG23 | 2.03 | 0.58 |
| 1:F:85:GLU:CB | 1:F:101:LEU:HD21 | 2.32 | 0.58 |
| 1:B:84:TRP:HA | 1:B:99:ASN:O | 2.03 | 0.58 |
| 2:H:227:VAL:HG21 | 2:H:248:LEU:HD12 | 1.84 | 0.58 |
| 1:F:171:LEU:N | 1:F:171:LEU:HD23 | 2.18 | 0.58 |
| 2:C:295:TYR:HD1 | 2:C:296:PRO:HD2 | 1.68 | 0.58 |
| 1:F:325:ASP:O | 1:F:327:LYS:HG3 | 2.03 | 0.58 |
| 1:E:194:TYR:CE1 | 1:E:204:VAL:HG22 | 2.39 | 0.58 |
| 2:C:334:ASP:O | 2:C:338:VAL:HG23 | 2.03 | 0.58 |
| 1:E:171:LEU:N | 1:E:171:LEU:HD23 | 2.18 | 0.58 |
| 1:A:84:TRP:HA | 1:A:99:ASN:O | 2.04 | 0.58 |
| 1:B:168:ASP:H | 1:B:188:LEU:HD23 | 1.68 | 0.58 |
| 2:G:451:LEU:CD2 | 2:G:458:ARG:HG3 | 2.33 | 0.58 |
| 1:E:325:ASP:O | 1:E:327:LYS:HG3 | 2.03 | 0.58 |
| 2:G:113:GLU:O | 2:G:116:ARG:HG2 | 2.04 | 0.58 |
| 2:C:274:LEU:HD22 | 2:C:281:SER:HB3 | 1.85 | 0.58 |
| 2:H:197:VAL:CG1 | 2:H:197:VAL:O | 2.52 | 0.58 |
| 1:A:171:LEU:HD23 | 1:A:171:LEU:N | 2.17 | 0.58 |
| 2:H:107:TYR:CZ | 2:H:111:LEU:HD11 | 2.38 | 0.58 |
| 2:D:454:LEU:CD2 | 2:D:503:VAL:HG21 | 2.33 | 0.58 |
| 2:H:274:LEU:HD22 | 2:H:281:SER:HB3 | 1.85 | 0.58 |
| 1:E:31:GLN:HG2 | 1:E:56:SER:O | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:227:VAL:HG21 | 2:D:248:LEU:HD12 | 1.86 | 0.58 |
| 2:G:394:CYS:O | 2:G:398:ILE:HG22 | 2.04 | 0.58 |
| 1:B:12:VAL:HA | 1:B:28:SER:CB | 2.34 | 0.58 |
| 1:F:85:GLU:HB2 | 1:F:101:LEU:HD11 | 1.86 | 0.58 |
| 2:C:521:TRP:CZ2 | 2:C:525:ILE:HD11 | 2.39 | 0.58 |
| 1:B:171:LEU:N | 1:B:171:LEU:HD23 | 2.18 | 0.58 |
| 1:A:213:SER:CB | 1:A:236:LYS:HB3 | 2.34 | 0.58 |
| 1:B:325:ASP:O | 1:B:327:LYS:HG3 | 2.03 | 0.58 |
| 2:D:334:ASP:O | 2:D:338:VAL:HG23 | 2.04 | 0.58 |
| 2:G:306:TRP:O | 2:G:310:VAL:HG23 | 2.03 | 0.57 |
| 2:D:262:ILE:HG23 | 2:D:289:ILE:HG23 | 1.86 | 0.57 |
| 1:A:231:ILE:CD1 | 1:A:245:ILE:HD11 | 2.34 | 0.57 |
| 1:E:214:LEU:HD12 | 1:E:214:LEU:N | 2.19 | 0.57 |
| 1:F:205:ALA:HB1 | 1:F:292:LEU:HD12 | 1.86 | 0.57 |
| 2:D:500:LYS:O | 2:D:504:ILE:HG13 | 2.03 | 0.57 |
| 2:H:459:ASN:N | 2:H:459:ASN:HD22 | 2.02 | 0.57 |
| 1:F:92:GLU:O | 1:F:93:CYS:HB2 | 2.04 | 0.57 |
| 2:H:186:ARG:HG3 | 2:H:190:PHE:HB2 | 1.87 | 0.57 |
| 2:G:42:PRO:HD3 | 2:G:48:LEU:CB | 2.27 | 0.57 |
| 2:H:299:SER:HB3 | 2:H:302:THR:OG1 | 2.04 | 0.57 |
| 2:G:406:LEU:HD22 | 2:G:421:ALA:HB2 | 1.86 | 0.57 |
| 2:H:508:LEU:HD11 | 2:H:522:MET:HG3 | 1.85 | 0.57 |
| 2:G:186:ARG:HG3 | 2:G:190:PHE:HB2 | 1.86 | 0.57 |
| 1:E:301:ASP:O | 1:E:303:HIS:N | 2.36 | 0.57 |
| 1:F:131:ASP:OD2 | 1:F:133:ILE:HD12 | 2.03 | 0.57 |
| 1:F:156:VAL:O | 1:F:157:LEU:HG | 2.03 | 0.57 |
| 2:C:482:TRP:N | 2:C:483:PRO:CD | 2.67 | 0.57 |
| 2:H:166:ASP:HB3 | 2:H:169:VAL:CG2 | 2.35 | 0.57 |
| 1:B:156:VAL:O | 1:B:157:LEU:HG | 2.04 | 0.57 |
| 1:A:183:LEU:HD12 | 1:A:184:ALA:N | 2.20 | 0.57 |
| 2:D:524:SER:O | 2:D:527:VAL:HB | 2.03 | 0.57 |
| 2:C:478:ASP:O | 2:C:480:GLU:N | 2.37 | 0.57 |
| 2:G:262:ILE:HG23 | 2:G:289:ILE:HG23 | 1.86 | 0.57 |
| 2:H:383:VAL:HG12 | 2:H:384:VAL:N | 2.20 | 0.57 |
| 1:E:176:SER:HB2 | 1:E:223:SER:OG | 2.05 | 0.57 |
| 2:C:42:PRO:HB3 | 2:C:46:ALA:C | 2.25 | 0.57 |
| 1:E:183:LEU:HD12 | 1:E:184:ALA:N | 2.20 | 0.57 |
| 1:E:156:VAL:O | 1:E:157:LEU:HG | 2.04 | 0.57 |
| 1:F:77:TYR:HD1 | 1:F:110:SER:HB2 | 1.68 | 0.57 |
| 2:D:515:THR:CG2 | 2:D:516:ASN:N | 2.67 | 0.57 |
| 1:A:26:THR:HG22 | 1:A:27:CYS:H | 1.68 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:270:LEU:HG | 2:H:271:LEU:N | 2.20 | 0.57 |
| 2:D:425:GLU:HB2 | 2:D:430:ILE:HD11 | 1.86 | 0.57 |
| 1:A:85:GLU:CB | 1:A:101:LEU:HD21 | 2.34 | 0.57 |
| 2:D:113:GLU:O | 2:D:116:ARG:HG2 | 2.05 | 0.57 |
| 1:A:226:ARG:HG3 | 1:A:226:ARG:HH11 | 1.70 | 0.57 |
| 2:H:42:PRO:HG3 | 2:H:48:LEU:HB2 | 1.86 | 0.57 |
| 2:H:285:VAL:O | 2:H:289:ILE:HG13 | 2.05 | 0.57 |
| 1:E:85:GLU:CB | 1:E:101:LEU:HD21 | 2.35 | 0.57 |
| 2:C:523:LEU:HD23 | 2:C:538:ILE:HD12 | 1.86 | 0.57 |
| 2:C:113:GLU:O | 2:C:116:ARG:HG2 | 2.05 | 0.57 |
| 1:A:205:ALA:HB1 | 1:A:292:LEU:HD12 | 1.87 | 0.57 |
| 1:B:176:SER:HB2 | 1:B:223:SER:OG | 2.04 | 0.57 |
| 1:F:84:TRP:HA | 1:F:99:ASN:O | 2.04 | 0.57 |
| 1:B:231:ILE:CD1 | 1:B:245:ILE:HD11 | 2.35 | 0.57 |
| 2:G:405:ILE:HG13 | 2:G:406:LEU:N | 2.20 | 0.57 |
| 1:F:117:ALA:HB2 | 1:F:173:TRP:CZ2 | 2.40 | 0.57 |
| 1:A:156:VAL:O | 1:A:157:LEU:HG | 2.05 | 0.57 |
| 1:A:38:LEU:HD21 | 2:C:77:GLN:HG3 | 1.85 | 0.57 |
| 1:A:145:LEU:H | 1:A:145:LEU:HD12 | 1.69 | 0.56 |
| 2:C:496:THR:HG22 | 2:C:497:ARG:N | 2.20 | 0.56 |
| 2:C:197:VAL:O | 2:C:197:VAL:CG1 | 2.53 | 0.56 |
| 2:C:394:CYS:O | 2:C:398:ILE:HG22 | 2.05 | 0.56 |
| 2:D:394:CYS:O | 2:D:398:ILE:HG22 | 2.05 | 0.56 |
| 1:A:176:SER:HB2 | 1:A:223:SER:OG | 2.05 | 0.56 |
| 2:D:453:ASP:CB | 2:D:456:SER:HB2 | 2.35 | 0.56 |
| 2:D:515:THR:HG22 | 2:D:516:ASN:N | 2.20 | 0.56 |
| 1:B:213:SER:CB | 1:B:236:LYS:HB3 | 2.35 | 0.56 |
| 2:G:425:GLU:HB2 | 2:G:430:ILE:HD11 | 1.87 | 0.56 |
| 1:A:214:LEU:N | 1:A:214:LEU:HD12 | 2.19 | 0.56 |
| 1:E:158:SER:C | 1:E:159:ILE:HD12 | 2.26 | 0.56 |
| 1:F:31:GLN:HG2 | 1:F:56:SER:O | 2.05 | 0.56 |
| 2:C:550:HIS:O | 2:C:553:ILE:HB | 2.05 | 0.56 |
| 2:H:454:LEU:HD13 | 2:H:495:GLY:HA3 | 1.87 | 0.56 |
| 2:H:402:ILE:CD1 | 2:H:429:LEU:HD13 | 2.36 | 0.56 |
| 1:E:121:LEU:HD21 | 1:E:181:GLU:HB2 | 1.88 | 0.56 |
| 2:G:500:LYS:O | 2:G:504:ILE:HG13 | 2.06 | 0.56 |
| 2:C:163:LYS:HE3 | 2:C:168:ARG:HH21 | 1.70 | 0.56 |
| 2:H:113:GLU:O | 2:H:116:ARG:HG2 | 2.05 | 0.56 |
| 2:D:42:PRO:CD | 2:D:48:LEU:N | 2.67 | 0.56 |
| 2:D:285:VAL:O | 2:D:289:ILE:HG13 | 2.05 | 0.56 |
| 2:C:270:LEU:HG | 2:C:271:LEU:N | 2.19 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:197:VAL:CG1 | 2:D:197:VAL:O | 2.54 | 0.56 |
| 2:C:534:ILE:O | 2:C:538:ILE:HG13 | 2.06 | 0.56 |
| 1:F:209:PRO:HG3 | 2:G:315:GLN:HA | 1.88 | 0.56 |
| 2:H:231:LYS:HE3 | 2:H:238:LYS:CG | 2.30 | 0.56 |
| 2:C:554:GLU:O | 2:C:558:ASN:N | 2.35 | 0.56 |
| 1:B:322:ALA:HB2 | 1:B:328:VAL:HG22 | 1.87 | 0.56 |
| 2:D:199:GLU:O | 2:D:199:GLU:HG2 | 2.06 | 0.56 |
| 1:B:194:TYR:CE1 | 1:B:204:VAL:HG22 | 2.40 | 0.56 |
| 2:C:393:PRO:O | 2:C:397:ILE:HG13 | 2.05 | 0.56 |
| 1:A:77:TYR:HD1 | 1:A:110:SER:HB2 | 1.69 | 0.56 |
| 1:B:26:THR:HG22 | 1:B:27:CYS:H | 1.70 | 0.56 |
| 2:H:240:PHE:HD2 | 2:H:268:SER:HB2 | 1.71 | 0.56 |
| 1:B:167:SER:HA | 1:B:188:LEU:HD21 | 1.88 | 0.56 |
| 2:C:186:ARG:HG3 | 2:C:190:PHE:HB2 | 1.88 | 0.56 |
| 1:A:228:TYR:HD2 | 1:A:244:LYS:HG3 | 1.71 | 0.56 |
| 2:G:296:PRO:CG | 2:G:302:THR:HG22 | 2.36 | 0.56 |
| 2:G:285:VAL:O | 2:G:289:ILE:HG13 | 2.06 | 0.56 |
| 1:A:209:PRO:HB2 | 2:D:318:GLY:HA3 | 1.88 | 0.56 |
| 1:A:57:SER:HB2 | 1:A:77:TYR:HD2 | 1.71 | 0.56 |
| 2:D:470:ALA:HA | 2:D:473:LEU:HD12 | 1.86 | 0.56 |
| 1:F:228:TYR:HD2 | 1:F:244:LYS:HG3 | 1.70 | 0.56 |
| 2:D:270:LEU:HG | 2:D:271:LEU:N | 2.20 | 0.56 |
| 2:C:262:ILE:HG23 | 2:C:289:ILE:HG23 | 1.88 | 0.56 |
| 1:B:158:SER:C | 1:B:159:ILE:HD12 | 2.26 | 0.56 |
| 2:D:393:PRO:O | 2:D:397:ILE:HG13 | 2.06 | 0.56 |
| 1:F:231:ILE:CD1 | 1:F:245:ILE:HD11 | 2.36 | 0.56 |
| 2:D:274:LEU:HD22 | 2:D:281:SER:HB3 | 1.88 | 0.56 |
| 1:F:71:ILE:HD11 | 1:F:145:LEU:CD2 | 2.36 | 0.56 |
| 1:E:312:TRP:CE2 | 1:E:319:LEU:HD13 | 2.41 | 0.56 |
| 2:H:496:THR:HG22 | 2:H:498:SER:H | 1.71 | 0.56 |
| 1:E:26:THR:HG22 | 1:E:27:CYS:H | 1.70 | 0.55 |
| 2:G:197:VAL:O | 2:G:197:VAL:CG1 | 2.52 | 0.55 |
| 2:H:391:GLU:O | 2:H:395:VAL:HG23 | 2.05 | 0.55 |
| 1:B:92:GLU:O | 1:B:93:CYS:HB2 | 2.06 | 0.55 |
| 2:H:515:THR:CG2 | 2:H:516:ASN:H | 2.16 | 0.55 |
| 2:G:295:TYR:HD1 | 2:G:296:PRO:HD2 | 1.72 | 0.55 |
| 2:G:240:PHE:HD2 | 2:G:268:SER:HB2 | 1.70 | 0.55 |
| 1:B:214:LEU:HD12 | 1:B:214:LEU:N | 2.20 | 0.55 |
| 2:G:492:SER:O | 2:G:494:THR:N | 2.38 | 0.55 |
| 1:A:111:LEU:HA | 1:A:129:GLY:HA2 | 1.89 | 0.55 |
| 1:F:26:THR:HG22 | 1:F:27:CYS:H | 1.70 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:296:PRO:CG | 2:D:302:THR:HG22 | 2.36 | 0.55 |
| 1:F:209:PRO:HB2 | 2:G:318:GLY:HA3 | 1.88 | 0.55 |
| 1:B:121:LEU:HD21 | 1:B:181:GLU:HB2 | 1.89 | 0.55 |
| 2:G:484:VAL:O | 2:G:488:LEU:HB2 | 2.05 | 0.55 |
| 1:F:121:LEU:HD21 | 1:F:181:GLU:HB2 | 1.87 | 0.55 |
| 1:F:145:LEU:HD12 | 1:F:145:LEU:H | 1.71 | 0.55 |
| 2:G:42:PRO:HD2 | 2:G:46:ALA:O | 2.07 | 0.55 |
| 2:H:406:LEU:HD22 | 2:H:421:ALA:HB2 | 1.88 | 0.55 |
| 1:E:334:THR:CG2 | 1:E:335:TYR:N | 2.70 | 0.55 |
| 1:A:335:TYR:HB3 | 2:D:373:GLU:HG3 | 1.88 | 0.55 |
| 1:B:77:TYR:HD1 | 1:B:110:SER:HB2 | 1.69 | 0.55 |
| 2:C:531:LEU:HD13 | 2:C:534:ILE:HD12 | 1.88 | 0.55 |
| 1:A:325:ASP:O | 1:A:327:LYS:HG3 | 2.06 | 0.55 |
| 2:D:486:ILE:HD12 | 2:D:504:ILE:HG23 | 1.89 | 0.55 |
| 1:B:57:SER:HB2 | 1:B:77:TYR:HD2 | 1.71 | 0.55 |
| 2:C:524:SER:O | 2:C:527:VAL:HB | 2.06 | 0.55 |
| 2:H:553:ILE:HA | 2:H:556:ILE:HG21 | 1.89 | 0.55 |
| 1:A:71:ILE:HD11 | 1:A:145:LEU:CD2 | 2.36 | 0.55 |
| 2:C:166:ASP:HB3 | 2:C:169:VAL:CG2 | 2.36 | 0.55 |
| 1:A:38:LEU:CD2 | 2:C:77:GLN:HG3 | 2.37 | 0.55 |
| 1:E:68:TYR:CG | 1:E:123:LEU:HD13 | 2.42 | 0.55 |
| 1:F:38:LEU:HD21 | 2:H:77:GLN:HG3 | 1.88 | 0.55 |
| 2:C:515:THR:HB | 2:C:518:ASP:OD1 | 2.06 | 0.55 |
| 2:H:295:TYR:HD1 | 2:H:296:PRO:HD2 | 1.70 | 0.55 |
| 1:E:322:ALA:HB2 | 1:E:328:VAL:HG22 | 1.88 | 0.55 |
| 2:H:68:LYS:HD2 | 2:H:81:PHE:HE1 | 1.71 | 0.55 |
| 2:G:393:PRO:O | 2:G:397:ILE:HG13 | 2.07 | 0.55 |
| 2:D:537:GLU:O | 2:D:540:THR:HB | 2.07 | 0.55 |
| 1:F:57:SER:HB2 | 1:F:77:TYR:HD2 | 1.71 | 0.55 |
| 2:G:199:GLU:O | 2:G:199:GLU:HG2 | 2.06 | 0.55 |
| 1:F:334:THR:CG2 | 1:F:335:TYR:N | 2.70 | 0.55 |
| 2:H:496:THR:HG22 | 2:H:497:ARG:N | 2.22 | 0.55 |
| 1:A:92:GLU:O | 1:A:93:CYS:HB2 | 2.07 | 0.55 |
| 2:D:484:VAL:O | 2:D:488:LEU:HB2 | 2.07 | 0.55 |
| 2:H:163:LYS:HE3 | 2:H:168:ARG:HH21 | 1.72 | 0.55 |
| 1:F:213:SER:CB | 1:F:236:LYS:HB3 | 2.36 | 0.54 |
| 1:E:224:ILE:HD12 | 1:E:315:THR:HA | 1.88 | 0.54 |
| 1:F:120:HIS:HB3 | 1:F:177:ARG:HG3 | 1.89 | 0.54 |
| 1:B:241:ARG:NH1 | 1:B:299:GLU:OE2 | 2.40 | 0.54 |
| 1:E:145:LEU:HD12 | 1:E:145:LEU:H | 1.72 | 0.54 |
| 2:D:197:VAL:HB | 2:D:366:PRO:HB2 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:306:TRP:O | 2:H:310:VAL:HG23 | 2.07 | 0.54 |
| 1:F:192:ILE:CG2 | 1:F:204:VAL:HG13 | 2.37 | 0.54 |
| 1:E:92:GLU:O | 1:E:93:CYS:HB2 | 2.06 | 0.54 |
| 1:B:96:ARG:HG2 | 1:B:96:ARG:HH11 | 1.71 | 0.54 |
| 2:C:240:PHE:HD2 | 2:C:268:SER:HB2 | 1.70 | 0.54 |
| 1:B:324:ASP:C | 1:B:326:GLY:H | 2.09 | 0.54 |
| 1:B:326:GLY:HA3 | 2:D:58:ILE:HD12 | 1.88 | 0.54 |
| 1:A:346:THR:OG1 | 1:A:347:ALA:N | 2.39 | 0.54 |
| 1:F:346:THR:OG1 | 1:F:347:ALA:N | 2.38 | 0.54 |
| 1:B:312:TRP:CE2 | 1:B:319:LEU:HD13 | 2.41 | 0.54 |
| 2:C:453:ASP:CB | 2:C:456:SER:HB2 | 2.37 | 0.54 |
| 2:C:425:GLU:HB2 | 2:C:430:ILE:HD11 | 1.89 | 0.54 |
| 1:E:336:SER:HA | 2:H:370:LEU:HD22 | 1.89 | 0.54 |
| 1:B:71:ILE:HD11 | 1:B:145:LEU:CD2 | 2.37 | 0.54 |
| 2:H:534:ILE:O | 2:H:538:ILE:HG13 | 2.08 | 0.54 |
| 2:D:379:LEU:HD22 | 2:D:384:VAL:HG22 | 1.90 | 0.54 |
| 2:H:394:CYS:O | 2:H:398:ILE:HG22 | 2.07 | 0.54 |
| 2:D:186:ARG:HG3 | 2:D:190:PHE:HB2 | 1.88 | 0.54 |
| 1:A:26:THR:HG22 | 1:A:27:CYS:N | 2.23 | 0.54 |
| 2:C:523:LEU:HD23 | 2:C:538:ILE:CD1 | 2.37 | 0.54 |
| 1:E:57:SER:HB2 | 1:E:77:TYR:HD2 | 1.72 | 0.54 |
| 1:F:104:LEU:HD13 | 1:F:137:TYR:CE2 | 2.42 | 0.54 |
| 1:B:336:SER:HA | 2:C:370:LEU:HD22 | 1.88 | 0.54 |
| 2:G:196:ASP:C | 2:G:198:GLU:H | 2.11 | 0.54 |
| 2:G:166:ASP:HB3 | 2:G:169:VAL:CG2 | 2.38 | 0.54 |
| 2:G:169:VAL:HG12 | 2:G:170:ASN:N | 2.23 | 0.54 |
| 1:A:85:GLU:HB2 | 1:A:101:LEU:HD11 | 1.88 | 0.54 |
| 1:F:181:GLU:OE1 | 1:F:196:ARG:HD3 | 2.07 | 0.54 |
| 2:G:52:THR:HG22 | 2:G:53:VAL:N | 2.23 | 0.54 |
| 2:C:405:ILE:HG13 | 2:C:406:LEU:N | 2.21 | 0.54 |
| 2:C:406:LEU:HD22 | 2:C:421:ALA:HB2 | 1.89 | 0.54 |
| 2:G:391:GLU:O | 2:G:395:VAL:HG23 | 2.07 | 0.54 |
| 2:H:379:LEU:HD22 | 2:H:384:VAL:HG22 | 1.90 | 0.54 |
| 2:G:163:LYS:HE3 | 2:G:168:ARG:HH21 | 1.73 | 0.54 |
| 2:H:199:GLU:O | 2:H:199:GLU:HG2 | 2.07 | 0.54 |
| 1:E:104:LEU:HD13 | 1:E:137:TYR:CE2 | 2.42 | 0.54 |
| 1:F:324:ASP:HB3 | 2:H:64:LYS:CG | 2.36 | 0.54 |
| 1:E:85:GLU:HB2 | 1:E:101:LEU:HD11 | 1.88 | 0.54 |
| 1:B:133:ILE:HG12 | 1:B:155:LYS:HG3 | 1.89 | 0.54 |
| 2:G:379:LEU:HD22 | 2:G:384:VAL:HG22 | 1.90 | 0.54 |
| 1:F:194:TYR:CE1 | 1:F:204:VAL:HG22 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:94:SER:OG | 1:A:95:GLY:N | 2.38 | 0.54 |
| 1:B:170:CYS:SG | 1:B:218:ILE:HG22 | 2.48 | 0.54 |
| 2:C:296:PRO:CG | 2:C:302:THR:HG22 | 2.37 | 0.54 |
| 2:H:405:ILE:HG13 | 2:H:406:LEU:N | 2.22 | 0.54 |
| 2:C:285:VAL:O | 2:C:289:ILE:HG13 | 2.08 | 0.54 |
| 1:B:334:THR:CG2 | 1:B:335:TYR:N | 2.70 | 0.54 |
| 1:B:38:LEU:HD21 | 2:D:77:GLN:HG3 | 1.89 | 0.54 |
| 2:D:163:LYS:HE3 | 2:D:168:ARG:HH21 | 1.72 | 0.54 |
| 2:C:52:THR:HG22 | 2:C:53:VAL:N | 2.23 | 0.54 |
| 2:C:486:ILE:HD12 | 2:C:504:ILE:HG23 | 1.90 | 0.54 |
| 2:G:344:ARG:CG | 2:G:344:ARG:HH11 | 2.21 | 0.54 |
| 2:D:429:LEU:O | 2:D:430:ILE:HG23 | 2.08 | 0.54 |
| 1:F:158:SER:C | 1:F:159:ILE:HD12 | 2.28 | 0.54 |
| 1:A:121:LEU:HD21 | 1:A:181:GLU:HB2 | 1.90 | 0.54 |
| 1:A:192:ILE:CG2 | 1:A:204:VAL:HG13 | 2.37 | 0.54 |
| 2:H:515:THR:CG2 | 2:H:516:ASN:N | 2.70 | 0.54 |
| 2:G:270:LEU:HG | 2:G:271:LEU:N | 2.23 | 0.54 |
| 2:D:406:LEU:HD22 | 2:D:421:ALA:HB2 | 1.89 | 0.54 |
| 2:H:393:PRO:O | 2:H:397:ILE:HG13 | 2.07 | 0.54 |
| 1:B:38:LEU:CD2 | 2:D:77:GLN:HG3 | 2.38 | 0.54 |
| 2:C:43:VAL:HG23 | 2:C:44:SER:N | 2.22 | 0.53 |
| 1:A:334:THR:CG2 | 1:A:335:TYR:N | 2.71 | 0.53 |
| 1:B:85:GLU:HB2 | 1:B:101:LEU:HD11 | 1.88 | 0.53 |
| 1:B:96:ARG:HG2 | 1:B:96:ARG:NH1 | 2.23 | 0.53 |
| 1:F:224:ILE:HD12 | 1:F:315:THR:HA | 1.90 | 0.53 |
| 1:B:111:LEU:HA | 1:B:129:GLY:HA2 | 1.91 | 0.53 |
| 2:C:556:ILE:HG22 | 2:C:557:ALA:N | 2.23 | 0.53 |
| 2:C:199:GLU:HG2 | 2:C:199:GLU:O | 2.08 | 0.53 |
| 1:E:326:GLY:HA3 | 2:G:58:ILE:HD12 | 1.90 | 0.53 |
| 2:D:240:PHE:HD2 | 2:D:268:SER:HB2 | 1.72 | 0.53 |
| 1:B:181:GLU:OE1 | 1:B:196:ARG:HD3 | 2.08 | 0.53 |
| 1:A:194:TYR:CE1 | 1:A:204:VAL:HG22 | 2.43 | 0.53 |
| 2:D:152:LEU:O | 2:D:156:GLU:HG3 | 2.09 | 0.53 |
| 2:H:52:THR:HG22 | 2:H:53:VAL:N | 2.22 | 0.53 |
| 2:H:270:LEU:HD13 | 2:H:289:ILE:HD12 | 1.90 | 0.53 |
| 2:D:274:LEU:HD11 | 2:D:285:VAL:HG21 | 1.88 | 0.53 |
| 2:D:52:THR:HG22 | 2:D:53:VAL:N | 2.23 | 0.53 |
| 2:D:158:PHE:O | 2:D:162:VAL:HG23 | 2.08 | 0.53 |
| 2:H:521:TRP:CH2 | 2:H:525:ILE:HD11 | 2.44 | 0.53 |
| 2:H:262:ILE:HG23 | 2:H:289:ILE:HG23 | 1.91 | 0.53 |
| 1:E:133:ILE:HG12 | 1:E:155:LYS:HG3 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:68:TYR:CG | 1:B:123:LEU:HD13 | 2.44 | 0.53 |
| 1:B:27:CYS:HB3 | 1:B:61:ILE:CD1 | 2.33 | 0.53 |
| 2:G:274:LEU:HD11 | 2:G:285:VAL:HG21 | 1.90 | 0.53 |
| 2:H:78:ASN:HB2 | 2:H:93:VAL:O | 2.08 | 0.53 |
| 2:H:196:ASP:C | 2:H:198:GLU:H | 2.12 | 0.53 |
| 1:E:241:ARG:NH1 | 1:E:241:ARG:HG2 | 2.23 | 0.53 |
| 2:D:166:ASP:HB3 | 2:D:169:VAL:CG2 | 2.39 | 0.53 |
| 1:A:158:SER:C | 1:A:159:ILE:HD12 | 2.29 | 0.53 |
| 1:A:128:LEU:HD22 | 1:A:185:VAL:CG1 | 2.38 | 0.53 |
| 2:H:124:PHE:HB2 | 2:H:426:ALA:O | 2.08 | 0.53 |
| 2:G:270:LEU:HD13 | 2:G:289:ILE:HD12 | 1.91 | 0.53 |
| 2:H:482:TRP:N | 2:H:483:PRO:CD | 2.72 | 0.53 |
| 2:C:402:ILE:CD1 | 2:C:429:LEU:HD13 | 2.39 | 0.53 |
| 1:A:181:GLU:OE1 | 1:A:196:ARG:HD3 | 2.09 | 0.53 |
| 1:E:86:GLU:HB2 | 1:E:98:TRP:CH2 | 2.44 | 0.53 |
| 1:F:26:THR:HG22 | 1:F:27:CYS:N | 2.24 | 0.53 |
| 2:C:306:TRP:O | 2:C:310:VAL:HG23 | 2.09 | 0.53 |
| 1:E:71:ILE:HD11 | 1:E:145:LEU:CD2 | 2.39 | 0.53 |
| 2:G:197:VAL:HB | 2:G:366:PRO:HB2 | 1.91 | 0.53 |
| 1:E:38:LEU:HD21 | 2:G:77:GLN:HG3 | 1.89 | 0.53 |
| 2:D:422:MET:SD | 2:D:423:ILE:N | 2.82 | 0.53 |
| 2:G:86:ASP:HA | 2:G:88:TYR:HE1 | 1.74 | 0.53 |
| 1:E:324:ASP:C | 1:E:326:GLY:H | 2.12 | 0.53 |
| 2:D:270:LEU:HD13 | 2:D:289:ILE:HD12 | 1.91 | 0.53 |
| 2:C:68:LYS:HD2 | 2:C:81:PHE:HE1 | 1.74 | 0.53 |
| 1:A:241:ARG:HG2 | 1:A:241:ARG:NH1 | 2.24 | 0.53 |
| 2:D:391:GLU:O | 2:D:395:VAL:HG23 | 2.09 | 0.53 |
| 2:G:103:GLU:H | 2:G:103:GLU:CD | 2.11 | 0.53 |
| 1:E:96:ARG:HG2 | 1:E:96:ARG:HH11 | 1.72 | 0.53 |
| 1:E:111:LEU:HA | 1:E:129:GLY:HA2 | 1.90 | 0.53 |
| 1:F:236:LYS:HG2 | 1:F:306:GLU:OE1 | 2.09 | 0.53 |
| 1:A:104:LEU:HD13 | 1:A:137:TYR:CE2 | 2.43 | 0.53 |
| 2:H:274:LEU:HD11 | 2:H:285:VAL:HG21 | 1.90 | 0.53 |
| 2:H:508:LEU:HB3 | 2:H:509:PRO:HD3 | 1.90 | 0.53 |
| 2:C:270:LEU:HD13 | 2:C:289:ILE:HD12 | 1.91 | 0.53 |
| 1:A:133:ILE:HG12 | 1:A:155:LYS:HG3 | 1.90 | 0.53 |
| 2:C:521:TRP:CE2 | 2:C:525:ILE:HD11 | 2.44 | 0.53 |
| 2:C:166:ASP:HB3 | 2:C:169:VAL:HG23 | 1.92 | 0.52 |
| 1:E:128:LEU:HD22 | 1:E:185:VAL:CG1 | 2.38 | 0.52 |
| 1:F:326:GLY:CA | 2:H:58:ILE:HD12 | 2.39 | 0.52 |
| 1:A:120:HIS:HB3 | 1:A:177:ARG:HG3 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:241:ARG:NH1 | 1:A:299:GLU:OE2 | 2.42 | 0.52 |
| 1:E:194:TYR:HE1 | 1:E:204:VAL:HG22 | 1.74 | 0.52 |
| 1:A:224:ILE:HD12 | 1:A:315:THR:HA | 1.91 | 0.52 |
| 2:C:43:VAL:HG23 | 2:C:44:SER:H | 1.74 | 0.52 |
| 1:E:213:SER:CB | 1:E:236:LYS:HB3 | 2.37 | 0.52 |
| 2:C:274:LEU:HD11 | 2:C:285:VAL:HG21 | 1.90 | 0.52 |
| 1:F:120:HIS:CB | 1:F:177:ARG:HG3 | 2.39 | 0.52 |
| 1:E:15:VAL:HG21 | 2:G:90:LEU:HD21 | 1.91 | 0.52 |
| 2:C:379:LEU:HD22 | 2:C:384:VAL:HG22 | 1.91 | 0.52 |
| 2:C:470:ALA:O | 2:C:473:LEU:HB2 | 2.09 | 0.52 |
| 1:E:26:THR:HG22 | 1:E:27:CYS:N | 2.23 | 0.52 |
| 2:H:453:ASP:CB | 2:H:456:SER:HB2 | 2.39 | 0.52 |
| 2:H:379:LEU:CD2 | 2:H:384:VAL:HG22 | 2.39 | 0.52 |
| 2:C:453:ASP:HB3 | 2:C:456:SER:HB2 | 1.90 | 0.52 |
| 1:B:128:LEU:HD22 | 1:B:185:VAL:CG1 | 2.39 | 0.52 |
| 2:C:152:LEU:O | 2:C:156:GLU:HG3 | 2.09 | 0.52 |
| 1:F:176:SER:HB2 | 1:F:223:SER:OG | 2.09 | 0.52 |
| 2:H:425:GLU:HB2 | 2:H:430:ILE:HD11 | 1.91 | 0.52 |
| 2:H:166:ASP:HB3 | 2:H:169:VAL:HG23 | 1.92 | 0.52 |
| 1:F:241:ARG:NH1 | 1:F:299:GLU:OE2 | 2.43 | 0.52 |
| 2:C:391:GLU:O | 2:C:395:VAL:HG23 | 2.09 | 0.52 |
| 1:F:190:GLN:O | 1:F:215:ILE:HD12 | 2.10 | 0.52 |
| 1:E:141:GLU:HG2 | 1:E:143:SER:OG | 2.08 | 0.52 |
| 2:H:308:ASN:C | 2:H:308:ASN:HD22 | 2.13 | 0.52 |
| 2:G:42:PRO:CG | 2:G:48:LEU:HB2 | 2.39 | 0.52 |
| 1:E:346:THR:OG1 | 1:E:347:ALA:N | 2.40 | 0.52 |
| 1:B:104:LEU:HD13 | 1:B:137:TYR:CE2 | 2.43 | 0.52 |
| 1:F:324:ASP:C | 1:F:326:GLY:H | 2.13 | 0.52 |
| 2:C:196:ASP:C | 2:C:198:GLU:H | 2.12 | 0.52 |
| 1:A:324:ASP:C | 1:A:326:GLY:H | 2.13 | 0.52 |
| 1:E:192:ILE:CG2 | 1:E:204:VAL:HG13 | 2.40 | 0.52 |
| 1:B:192:ILE:CG2 | 1:B:204:VAL:HG13 | 2.39 | 0.52 |
| 1:E:96:ARG:HG2 | 1:E:96:ARG:NH1 | 2.24 | 0.52 |
| 2:H:508:LEU:HD11 | 2:H:522:MET:CG | 2.40 | 0.52 |
| 2:G:204:PHE:HD1 | 2:G:205:ILE:N | 2.07 | 0.52 |
| 2:D:68:LYS:HD2 | 2:D:81:PHE:HE1 | 1.74 | 0.52 |
| 1:B:190:GLN:O | 1:B:215:ILE:HD12 | 2.09 | 0.52 |
| 1:F:141:GLU:HG2 | 1:F:143:SER:OG | 2.10 | 0.52 |
| 1:B:183:LEU:HD12 | 1:B:184:ALA:N | 2.24 | 0.52 |
| 1:F:322:ALA:HB2 | 1:F:328:VAL:HG22 | 1.91 | 0.52 |
| 2:C:533:GLU:OE1 | 2:C:533:GLU:HA | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:120:HIS:HB3 | 1:B:177:ARG:HG3 | 1.92 | 0.52 |
| 1:F:128:LEU:HD22 | 1:F:185:VAL:CG1 | 2.40 | 0.52 |
| 2:C:492:SER:O | 2:C:500:LYS:NZ | 2.37 | 0.52 |
| 1:A:190:GLN:O | 1:A:215:ILE:HD12 | 2.10 | 0.52 |
| 1:A:322:ALA:HB2 | 1:A:328:VAL:HG22 | 1.91 | 0.52 |
| 1:A:334:THR:HG22 | 1:A:335:TYR:H | 1.75 | 0.52 |
| 1:B:241:ARG:HG2 | 1:B:241:ARG:NH1 | 2.25 | 0.52 |
| 2:D:379:LEU:CD2 | 2:D:384:VAL:HG22 | 2.40 | 0.52 |
| 2:C:379:LEU:HD11 | 2:C:395:VAL:CG1 | 2.40 | 0.52 |
| 1:F:38:LEU:CD2 | 2:H:77:GLN:HG3 | 2.39 | 0.52 |
| 2:D:295:TYR:HD1 | 2:D:296:PRO:HD2 | 1.74 | 0.51 |
| 1:F:324:ASP:HB3 | 2:H:64:LYS:HB3 | 1.92 | 0.51 |
| 2:H:272:PRO:O | 2:H:273:TYR:C | 2.49 | 0.51 |
| 1:A:120:HIS:CB | 1:A:177:ARG:HG3 | 2.40 | 0.51 |
| 2:D:204:PHE:HD1 | 2:D:205:ILE:N | 2.08 | 0.51 |
| 2:H:296:PRO:CG | 2:H:302:THR:HG22 | 2.37 | 0.51 |
| 2:D:196:ASP:C | 2:D:198:GLU:H | 2.13 | 0.51 |
| 1:E:329:ARG:NH1 | 2:G:44:SER:HB2 | 2.25 | 0.51 |
| 1:B:224:ILE:HD12 | 1:B:315:THR:HA | 1.91 | 0.51 |
| 2:H:152:LEU:O | 2:H:156:GLU:HG3 | 2.10 | 0.51 |
| 2:G:379:LEU:CD2 | 2:G:384:VAL:HG22 | 2.40 | 0.51 |
| 1:B:346:THR:OG1 | 1:B:347:ALA:N | 2.41 | 0.51 |
| 2:H:103:GLU:CD | 2:H:103:GLU:H | 2.13 | 0.51 |
| 2:H:335:PHE:CD2 | 2:H:339:ILE:HD11 | 2.46 | 0.51 |
| 1:F:214:LEU:H | 1:F:214:LEU:CD1 | 2.22 | 0.51 |
| 2:C:192:LEU:HD11 | 2:C:204:PHE:HD2 | 1.76 | 0.51 |
| 2:D:453:ASP:HB2 | 2:D:456:SER:HB2 | 1.91 | 0.51 |
| 2:G:537:GLU:O | 2:G:540:THR:HB | 2.10 | 0.51 |
| 2:D:42:PRO:CD | 2:D:47:ILE:C | 2.79 | 0.51 |
| 1:B:26:THR:HG22 | 1:B:27:CYS:N | 2.25 | 0.51 |
| 2:D:86:ASP:HA | 2:D:88:TYR:HE1 | 1.75 | 0.51 |
| 2:C:429:LEU:O | 2:C:430:ILE:HG23 | 2.11 | 0.51 |
| 2:D:78:ASN:HB2 | 2:D:93:VAL:O | 2.11 | 0.51 |
| 1:F:94:SER:OG | 1:F:95:GLY:N | 2.41 | 0.51 |
| 2:H:461:MET:O | 2:H:465:MET:HG3 | 2.11 | 0.51 |
| 2:D:97:ARG:HD2 | 2:D:174:GLU:OE2 | 2.11 | 0.51 |
| 1:A:136:LEU:HD11 | 1:A:202:LEU:HD11 | 1.93 | 0.51 |
| 2:G:429:LEU:O | 2:G:430:ILE:HG23 | 2.11 | 0.51 |
| 2:D:534:ILE:O | 2:D:538:ILE:HG13 | 2.10 | 0.51 |
| 1:F:133:ILE:HG12 | 1:F:155:LYS:HG3 | 1.92 | 0.51 |
| 1:E:94:SER:OG | 1:E:95:GLY:N | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:10:ASP:C | 2:D:88:TYR:HE2 | 2.14 | 0.51 |
| 2:D:322:THR:HG23 | 2:D:324:ILE:HG12 | 1.92 | 0.51 |
| 1:B:334:THR:HG22 | 1:B:335:TYR:H | 1.75 | 0.51 |
| 1:F:241:ARG:HG2 | 1:F:241:ARG:NH1 | 2.26 | 0.51 |
| 2:G:369:GLU:HG2 | 2:H:457:TYR:O | 2.11 | 0.51 |
| 1:E:190:GLN:O | 1:E:215:ILE:HD12 | 2.11 | 0.51 |
| 1:B:94:SER:OG | 1:B:95:GLY:N | 2.44 | 0.51 |
| 1:B:86:GLU:HB2 | 1:B:98:TRP:CH2 | 2.46 | 0.51 |
| 2:D:42:PRO:CB | 2:D:48:LEU:HD22 | 2.27 | 0.51 |
| 2:D:335:PHE:CD2 | 2:D:339:ILE:HD11 | 2.46 | 0.51 |
| 1:A:108:LYS:HE2 | 1:A:133:ILE:CD1 | 2.40 | 0.51 |
| 1:E:221:ALA:HB2 | 1:E:312:TRP:CE2 | 2.46 | 0.51 |
| 1:E:34:LYS:HE2 | 1:E:50:SER:OG | 2.11 | 0.51 |
| 1:B:228:TYR:HD2 | 1:B:244:LYS:HG3 | 1.76 | 0.51 |
| 2:C:56:GLN:HG3 | 2:C:56:GLN:O | 2.11 | 0.51 |
| 2:D:367:SER:C | 2:D:369:GLU:H | 2.14 | 0.51 |
| 2:D:42:PRO:HB3 | 2:D:48:LEU:CG | 2.40 | 0.50 |
| 1:E:245:ILE:HA | 1:E:293:GLN:O | 2.11 | 0.50 |
| 2:C:231:LYS:H | 2:C:234:THR:HB | 1.75 | 0.50 |
| 1:E:241:ARG:NH1 | 1:E:299:GLU:OE2 | 2.43 | 0.50 |
| 2:G:235:ALA:C | 2:G:237:LYS:H | 2.14 | 0.50 |
| 2:G:158:PHE:O | 2:G:162:VAL:HG23 | 2.11 | 0.50 |
| 2:C:103:GLU:H | 2:C:103:GLU:CD | 2.14 | 0.50 |
| 2:G:513:PHE:C | 2:G:513:PHE:CD1 | 2.85 | 0.50 |
| 1:E:310:VAL:O | 1:E:310:VAL:HG13 | 2.11 | 0.50 |
| 1:E:228:TYR:HD2 | 1:E:244:LYS:HG3 | 1.77 | 0.50 |
| 1:A:236:LYS:HG2 | 1:A:306:GLU:OE1 | 2.11 | 0.50 |
| 1:A:336:SER:HA | 2:D:370:LEU:HD22 | 1.94 | 0.50 |
| 2:C:508:LEU:HB3 | 2:C:509:PRO:HD3 | 1.94 | 0.50 |
| 2:G:481:LEU:O | 2:G:484:VAL:HB | 2.12 | 0.50 |
| 2:C:373:GLU:O | 2:C:377:MET:HG3 | 2.12 | 0.50 |
| 2:C:423:ILE:O | 2:C:426:ALA:HB3 | 2.11 | 0.50 |
| 1:F:34:LYS:HE2 | 1:F:50:SER:OG | 2.12 | 0.50 |
| 1:E:231:ILE:HD11 | 1:E:245:ILE:HD11 | 1.93 | 0.50 |
| 1:B:108:LYS:HE2 | 1:B:133:ILE:CD1 | 2.41 | 0.50 |
| 2:G:422:MET:SD | 2:G:423:ILE:N | 2.85 | 0.50 |
| 2:D:246:TRP:CE2 | 2:D:331:TYR:HB3 | 2.47 | 0.50 |
| 2:C:367:SER:C | 2:C:369:GLU:H | 2.15 | 0.50 |
| 1:F:295:GLU:HG2 | 2:G:311:LEU:HD21 | 1.94 | 0.50 |
| 2:C:557:ALA:O | 2:C:561:ARG:N | 2.39 | 0.50 |
| 2:C:375:LEU:HD11 | 2:C:395:VAL:HG13 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:246:TRP:CE2 | 2:G:331:TYR:HB3 | 2.47 | 0.50 |
| 2:H:492:SER:O | 2:H:500:LYS:NZ | 2.41 | 0.50 |
| 2:G:514:VAL:HG12 | 2:G:515:THR:N | 2.27 | 0.50 |
| 2:C:158:PHE:O | 2:C:162:VAL:HG23 | 2.12 | 0.50 |
| 2:D:103:GLU:CD | 2:D:103:GLU:H | 2.15 | 0.50 |
| 2:D:42:PRO:HD2 | 2:D:47:ILE:CA | 2.42 | 0.50 |
| 2:C:204:PHE:HD1 | 2:C:205:ILE:N | 2.09 | 0.50 |
| 2:G:152:LEU:O | 2:G:156:GLU:HG3 | 2.12 | 0.50 |
| 1:B:34:LYS:HE2 | 1:B:50:SER:OG | 2.12 | 0.50 |
| 2:H:344:ARG:CG | 2:H:344:ARG:HH11 | 2.21 | 0.50 |
| 2:D:271:LEU:N | 2:D:272:PRO:CD | 2.75 | 0.50 |
| 2:C:169:VAL:HG12 | 2:C:170:ASN:N | 2.27 | 0.50 |
| 2:C:379:LEU:CD2 | 2:C:384:VAL:HG22 | 2.42 | 0.50 |
| 1:E:38:LEU:CD2 | 2:G:77:GLN:HG3 | 2.41 | 0.50 |
| 2:D:169:VAL:HG12 | 2:D:170:ASN:N | 2.25 | 0.49 |
| 1:F:221:ALA:HB2 | 1:F:312:TRP:CE2 | 2.47 | 0.49 |
| 2:G:451:LEU:CD1 | 2:G:458:ARG:HG3 | 2.42 | 0.49 |
| 2:H:379:LEU:HD11 | 2:H:395:VAL:CG1 | 2.42 | 0.49 |
| 2:D:190:PHE:CZ | 2:D:427:LYS:HG3 | 2.47 | 0.49 |
| 2:G:214:ARG:O | 2:G:214:ARG:HG3 | 2.12 | 0.49 |
| 1:A:96:ARG:HG2 | 1:A:96:ARG:NH1 | 2.27 | 0.49 |
| 2:G:322:THR:HG23 | 2:G:324:ILE:HG12 | 1.92 | 0.49 |
| 2:H:482:TRP:O | 2:H:486:ILE:HG12 | 2.12 | 0.49 |
| 2:H:429:LEU:O | 2:H:430:ILE:HG23 | 2.12 | 0.49 |
| 2:G:166:ASP:HB3 | 2:G:169:VAL:HG23 | 1.94 | 0.49 |
| 1:E:120:HIS:HB3 | 1:E:177:ARG:HG3 | 1.94 | 0.49 |
| 2:G:68:LYS:HD2 | 2:G:81:PHE:HE1 | 1.77 | 0.49 |
| 1:B:194:TYR:HE1 | 1:B:204:VAL:HG22 | 1.77 | 0.49 |
| 2:H:94:ARG:HH21 | 2:H:98:LEU:HB3 | 1.76 | 0.49 |
| 2:H:98:LEU:HD11 | 2:H:476:LEU:CD1 | 2.42 | 0.49 |
| 2:D:214:ARG:HG3 | 2:D:214:ARG:O | 2.11 | 0.49 |
| 1:F:194:TYR:HE1 | 1:F:204:VAL:HG22 | 1.77 | 0.49 |
| 1:B:141:GLU:HG2 | 1:B:143:SER:OG | 2.12 | 0.49 |
| 2:C:173:TYR:HA | 2:C:176:GLU:HB2 | 1.93 | 0.49 |
| 2:D:56:GLN:O | 2:D:56:GLN:HG3 | 2.11 | 0.49 |
| 2:G:367:SER:C | 2:G:369:GLU:H | 2.15 | 0.49 |
| 1:A:221:ALA:HB2 | 1:A:312:TRP:CE2 | 2.47 | 0.49 |
| 1:E:128:LEU:HD22 | 1:E:185:VAL:HG11 | 1.94 | 0.49 |
| 1:A:86:GLU:HB2 | 1:A:98:TRP:CH2 | 2.47 | 0.49 |
| 2:G:334:ASP:O | 2:G:338:VAL:HG23 | 2.10 | 0.49 |
| 2:H:367:SER:C | 2:H:369:GLU:H | 2.16 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:27:CYS:HB3 | 1:E:61:ILE:CD1 | 2.37 | 0.49 |
| 1:B:245:ILE:HA | 1:B:293:GLN:O | 2.11 | 0.49 |
| 2:C:69:PHE:CD2 | 2:C:80:ALA:HB2 | 2.47 | 0.49 |
| 2:C:69:PHE:HD2 | 2:C:80:ALA:HB2 | 1.76 | 0.49 |
| 2:G:192:LEU:HD11 | 2:G:204:PHE:HD2 | 1.77 | 0.49 |
| 1:B:221:ALA:HB2 | 1:B:312:TRP:CE2 | 2.47 | 0.49 |
| 1:A:194:TYR:HE1 | 1:A:204:VAL:HG22 | 1.78 | 0.49 |
| 2:G:227:VAL:HG21 | 2:G:248:LEU:HD12 | 1.93 | 0.49 |
| 2:C:42:PRO:HA | 2:C:46:ALA:O | 2.13 | 0.49 |
| 2:C:482:TRP:N | 2:C:483:PRO:HD3 | 2.25 | 0.49 |
| 2:C:268:SER:O | 2:C:272:PRO:HD2 | 2.12 | 0.49 |
| 1:A:141:GLU:HG2 | 1:A:143:SER:OG | 2.12 | 0.49 |
| 1:F:136:LEU:HD11 | 1:F:202:LEU:HD11 | 1.94 | 0.49 |
| 2:D:86:ASP:N | 2:D:88:TYR:CE1 | 2.80 | 0.49 |
| 2:C:86:ASP:HA | 2:C:88:TYR:HE1 | 1.77 | 0.49 |
| 2:H:155:LEU:O | 2:H:159:ILE:HG13 | 2.13 | 0.49 |
| 2:G:86:ASP:HA | 2:G:88:TYR:CE1 | 2.48 | 0.49 |
| 2:C:335:PHE:CD2 | 2:C:339:ILE:HD11 | 2.48 | 0.49 |
| 1:F:334:THR:HG22 | 1:F:335:TYR:H | 1.75 | 0.49 |
| 1:B:120:HIS:CB | 1:B:177:ARG:HG3 | 2.43 | 0.49 |
| 2:H:231:LYS:HG3 | 2:H:232:ASP:N | 2.27 | 0.49 |
| 2:G:69:PHE:HD2 | 2:G:80:ALA:HB2 | 1.76 | 0.49 |
| 2:D:272:PRO:O | 2:D:273:TYR:C | 2.50 | 0.49 |
| 2:H:549:ALA:O | 2:H:551:ASN:N | 2.45 | 0.49 |
| 2:D:166:ASP:HB3 | 2:D:169:VAL:HG23 | 1.95 | 0.49 |
| 2:H:398:ILE:HG23 | 2:H:399:SER:N | 2.28 | 0.49 |
| 1:A:193:ILE:CD1 | 1:A:245:ILE:HD13 | 2.43 | 0.49 |
| 2:D:423:ILE:O | 2:D:426:ALA:HB3 | 2.12 | 0.49 |
| 1:B:236:LYS:HG2 | 1:B:306:GLU:OE1 | 2.13 | 0.49 |
| 1:E:11:LEU:N | 2:G:88:TYR:HE2 | 2.10 | 0.49 |
| 1:E:236:LYS:HG2 | 1:E:306:GLU:OE1 | 2.12 | 0.49 |
| 2:C:272:PRO:O | 2:C:273:TYR:C | 2.51 | 0.49 |
| 2:H:104:PHE:O | 2:H:107:TYR:N | 2.46 | 0.49 |
| 1:A:247:GLU:HB3 | 1:A:292:LEU:HD23 | 1.94 | 0.49 |
| 2:H:231:LYS:NZ | 2:H:238:LYS:HD3 | 2.28 | 0.48 |
| 1:F:231:ILE:HD11 | 1:F:245:ILE:HD11 | 1.95 | 0.48 |
| 2:C:535:ALA:HA | 2:C:538:ILE:HD12 | 1.95 | 0.48 |
| 1:A:128:LEU:HD22 | 1:A:185:VAL:HG11 | 1.95 | 0.48 |
| 1:F:79:LYS:HG2 | 1:F:110:SER:N | 2.27 | 0.48 |
| 1:A:79:LYS:HG2 | 1:A:110:SER:N | 2.28 | 0.48 |
| 2:H:344:ARG:HG3 | 2:H:344:ARG:NH1 | 2.25 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:168:ASP:H | 1:F:188:LEU:CD2 | 2.26 | 0.48 |
| 2:H:204:PHE:O | 2:H:206:GLU:N | 2.46 | 0.48 |
| 2:H:158:PHE:O | 2:H:162:VAL:HG23 | 2.12 | 0.48 |
| 1:A:208:LEU:HD11 | 1:A:231:ILE:HD12 | 1.94 | 0.48 |
| 2:C:515:THR:HG22 | 2:C:517:ASP:N | 2.20 | 0.48 |
| 2:H:173:TYR:HA | 2:H:176:GLU:HB2 | 1.95 | 0.48 |
| 1:A:114:VAL:HG23 | 1:A:126:ALA:O | 2.13 | 0.48 |
| 2:G:515:THR:HG22 | 2:G:517:ASP:N | 2.22 | 0.48 |
| 2:H:268:SER:O | 2:H:272:PRO:HD2 | 2.13 | 0.48 |
| 2:G:552:ILE:HG22 | 2:G:552:ILE:O | 2.13 | 0.48 |
| 1:B:247:GLU:HB3 | 1:B:292:LEU:HD23 | 1.95 | 0.48 |
| 1:A:68:TYR:CG | 1:A:123:LEU:HD13 | 2.49 | 0.48 |
| 2:G:69:PHE:CD2 | 2:G:80:ALA:HB2 | 2.49 | 0.48 |
| 1:E:334:THR:HG22 | 1:E:335:TYR:H | 1.74 | 0.48 |
| 1:A:138:ASP:HA | 1:A:148:TRP:CE3 | 2.49 | 0.48 |
| 2:G:56:GLN:O | 2:G:56:GLN:HG3 | 2.13 | 0.48 |
| 2:C:322:THR:HG23 | 2:C:324:ILE:HG12 | 1.95 | 0.48 |
| 2:D:98:LEU:HD12 | 2:D:99:ASP:H | 1.78 | 0.48 |
| 1:E:181:GLU:OE1 | 1:E:196:ARG:HD3 | 2.13 | 0.48 |
| 2:H:189:TYR:O | 2:H:427:LYS:HE3 | 2.14 | 0.48 |
| 2:H:56:GLN:HG3 | 2:H:56:GLN:O | 2.13 | 0.48 |
| 1:E:324:ASP:HB3 | 2:G:64:LYS:CG | 2.42 | 0.48 |
| 2:C:532:PRO:HG2 | 2:C:533:GLU:H | 1.78 | 0.48 |
| 1:E:214:LEU:H | 1:E:214:LEU:CD1 | 2.25 | 0.48 |
| 1:F:128:LEU:HD22 | 1:F:185:VAL:HG11 | 1.96 | 0.48 |
| 1:F:247:GLU:HB3 | 1:F:292:LEU:HD23 | 1.94 | 0.48 |
| 1:A:247:GLU:HB3 | 1:A:292:LEU:CD2 | 2.44 | 0.48 |
| 2:D:145:ASN:OD1 | 2:D:190:PHE:HA | 2.14 | 0.48 |
| 2:D:308:ASN:HD22 | 2:D:308:ASN:C | 2.16 | 0.48 |
| 1:B:310:VAL:HG13 | 1:B:310:VAL:O | 2.14 | 0.48 |
| 2:D:478:ASP:O | 2:D:480:GLU:N | 2.47 | 0.48 |
| 2:C:344:ARG:CG | 2:C:344:ARG:HH11 | 2.20 | 0.48 |
| 2:D:344:ARG:HG3 | 2:D:344:ARG:NH1 | 2.26 | 0.48 |
| 2:G:398:ILE:HG23 | 2:G:399:SER:N | 2.29 | 0.48 |
| 1:A:15:VAL:O | 2:C:70:LYS:HD2 | 2.13 | 0.48 |
| 2:C:308:ASN:HD22 | 2:C:308:ASN:C | 2.16 | 0.48 |
| 2:G:523:LEU:HD23 | 2:G:538:ILE:CD1 | 2.43 | 0.48 |
| 1:B:231:ILE:HD11 | 1:B:245:ILE:HD11 | 1.94 | 0.48 |
| 2:D:268:SER:O | 2:D:272:PRO:HD2 | 2.13 | 0.48 |
| 2:H:169:VAL:HG12 | 2:H:170:ASN:N | 2.27 | 0.48 |
| 1:B:247:GLU:HB3 | 1:B:292:LEU:CD2 | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:224:ILE:HG22 | 2:D:471:PHE:CZ | 2.48 | 0.48 |
| 1:A:96:ARG:HG2 | 1:A:96:ARG:HH11 | 1.78 | 0.48 |
| 1:F:86:GLU:HB2 | 1:F:98:TRP:CH2 | 2.48 | 0.48 |
| 2:C:271:LEU:N | 2:C:272:PRO:CD | 2.77 | 0.48 |
| 2:C:508:LEU:HD11 | 2:C:522:MET:HG3 | 1.96 | 0.48 |
| 2:D:204:PHE:O | 2:D:206:GLU:N | 2.47 | 0.48 |
| 1:E:226:ARG:NH1 | 1:E:226:ARG:HG3 | 2.28 | 0.48 |
| 2:G:78:ASN:HB2 | 2:G:93:VAL:O | 2.13 | 0.48 |
| 2:H:471:PHE:O | 2:H:473:LEU:N | 2.47 | 0.48 |
| 2:H:459:ASN:HB3 | 2:H:494:THR:CB | 2.44 | 0.48 |
| 2:G:190:PHE:CZ | 2:G:427:LYS:HG3 | 2.48 | 0.48 |
| 2:D:398:ILE:HG23 | 2:D:399:SER:N | 2.29 | 0.48 |
| 1:F:151:THR:HG22 | 1:F:152:SER:N | 2.29 | 0.48 |
| 2:H:52:THR:HG22 | 2:H:54:ASN:H | 1.79 | 0.48 |
| 2:H:422:MET:SD | 2:H:423:ILE:N | 2.87 | 0.48 |
| 2:C:155:LEU:O | 2:C:159:ILE:HG13 | 2.13 | 0.48 |
| 1:F:96:ARG:NH1 | 1:F:96:ARG:HG2 | 2.29 | 0.48 |
| 1:E:193:ILE:CD1 | 1:E:245:ILE:HD13 | 2.44 | 0.47 |
| 2:G:268:SER:O | 2:G:272:PRO:HD2 | 2.13 | 0.47 |
| 1:E:54:HIS:HD2 | 1:E:58:ILE:HG12 | 1.78 | 0.47 |
| 1:B:214:LEU:H | 1:B:214:LEU:CD1 | 2.25 | 0.47 |
| 2:H:192:LEU:HD11 | 2:H:204:PHE:HD2 | 1.75 | 0.47 |
| 2:D:52:THR:HG22 | 2:D:54:ASN:H | 1.79 | 0.47 |
| 2:C:86:ASP:HA | 2:C:88:TYR:CE1 | 2.49 | 0.47 |
| 2:G:173:TYR:HA | 2:G:176:GLU:HB2 | 1.95 | 0.47 |
| 2:D:313:LEU:C | 2:D:313:LEU:HD23 | 2.35 | 0.47 |
| 2:G:86:ASP:N | 2:G:88:TYR:CE1 | 2.82 | 0.47 |
| 2:H:69:PHE:HD2 | 2:H:80:ALA:HB2 | 1.79 | 0.47 |
| 1:F:54:HIS:CE1 | 1:F:82:LYS:HB2 | 2.49 | 0.47 |
| 1:E:247:GLU:HB3 | 1:E:292:LEU:HD23 | 1.96 | 0.47 |
| 1:F:108:LYS:HE2 | 1:F:133:ILE:CD1 | 2.44 | 0.47 |
| 2:G:469:PHE:O | 2:G:472:GLU:N | 2.47 | 0.47 |
| 2:G:117:ASP:C | 2:G:119:GLY:H | 2.18 | 0.47 |
| 2:G:505:ALA:HB2 | 2:G:531:LEU:HD22 | 1.95 | 0.47 |
| 1:E:120:HIS:CB | 1:E:177:ARG:HG3 | 2.44 | 0.47 |
| 1:E:247:GLU:HB3 | 1:E:292:LEU:CD2 | 2.45 | 0.47 |
| 1:E:108:LYS:HE2 | 1:E:133:ILE:CD1 | 2.43 | 0.47 |
| 2:C:52:THR:HG22 | 2:C:54:ASN:H | 1.79 | 0.47 |
| 2:H:153:ASN:O | 2:H:156:GLU:N | 2.46 | 0.47 |
| 2:D:118:LEU:O | 2:D:119:GLY:C | 2.53 | 0.47 |
| 2:D:502:MET:O | 2:D:505:ALA:HB3 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:269:ASP:O | 2:G:270:LEU:C | 2.53 | 0.47 |
| 2:G:271:LEU:N | 2:G:272:PRO:CD | 2.77 | 0.47 |
| 2:H:204:PHE:HD1 | 2:H:205:ILE:N | 2.12 | 0.47 |
| 2:H:470:ALA:O | 2:H:473:LEU:HB2 | 2.15 | 0.47 |
| 1:F:247:GLU:HB3 | 1:F:292:LEU:CD2 | 2.44 | 0.47 |
| 1:B:128:LEU:HD22 | 1:B:185:VAL:HG11 | 1.97 | 0.47 |
| 2:G:250:ASN:O | 2:G:254:LEU:HG | 2.13 | 0.47 |
| 2:D:86:ASP:HA | 2:D:88:TYR:CE1 | 2.49 | 0.47 |
| 2:G:240:PHE:HD2 | 2:G:268:SER:CB | 2.28 | 0.47 |
| 2:H:532:PRO:O | 2:H:535:ALA:HB3 | 2.15 | 0.47 |
| 2:D:198:GLU:HA | 2:D:300:SER:OG | 2.14 | 0.47 |
| 2:C:204:PHE:O | 2:C:206:GLU:N | 2.48 | 0.47 |
| 2:G:204:PHE:O | 2:G:206:GLU:N | 2.48 | 0.47 |
| 1:F:96:ARG:HH11 | 1:F:96:ARG:HG2 | 1.80 | 0.47 |
| 2:G:118:LEU:O | 2:G:119:GLY:C | 2.52 | 0.47 |
| 1:F:310:VAL:HG13 | 1:F:310:VAL:O | 2.15 | 0.47 |
| 2:C:42:PRO:HB3 | 2:C:46:ALA:O | 2.14 | 0.47 |
| 1:A:310:VAL:HG13 | 1:A:310:VAL:O | 2.15 | 0.47 |
| 2:D:228:PHE:CE2 | 2:D:267:ARG:HG3 | 2.49 | 0.47 |
| 2:G:112:PHE:O | 2:G:115:TYR:HB3 | 2.14 | 0.47 |
| 2:H:184:CYS:HB2 | 2:H:211:TRP:CE2 | 2.49 | 0.47 |
| 2:H:322:THR:HG23 | 2:H:324:ILE:HG12 | 1.95 | 0.47 |
| 2:D:269:ASP:O | 2:D:270:LEU:C | 2.52 | 0.47 |
| 1:A:324:ASP:HB3 | 2:C:64:LYS:CG | 2.43 | 0.47 |
| 2:G:505:ALA:HB2 | 2:G:531:LEU:CD2 | 2.45 | 0.47 |
| 1:A:214:LEU:CD1 | 1:A:214:LEU:H | 2.26 | 0.47 |
| 2:D:104:PHE:O | 2:D:107:TYR:N | 2.47 | 0.47 |
| 2:D:104:PHE:C | 2:D:106:ALA:H | 2.18 | 0.47 |
| 2:H:98:LEU:HD12 | 2:H:99:ASP:H | 1.79 | 0.47 |
| 2:G:155:LEU:O | 2:G:159:ILE:HG13 | 2.14 | 0.47 |
| 1:A:97:ARG:HG3 | 1:A:97:ARG:HH11 | 1.80 | 0.47 |
| 1:F:68:TYR:CG | 1:F:123:LEU:HD13 | 2.49 | 0.47 |
| 2:D:155:LEU:O | 2:D:159:ILE:HG13 | 2.14 | 0.47 |
| 1:A:231:ILE:HD11 | 1:A:245:ILE:HD11 | 1.96 | 0.47 |
| 2:G:335:PHE:CD2 | 2:G:339:ILE:HD11 | 2.50 | 0.47 |
| 2:H:271:LEU:O | 2:H:275:SER:HB3 | 2.15 | 0.47 |
| 2:H:375:LEU:HD11 | 2:H:395:VAL:HG13 | 1.96 | 0.47 |
| 2:D:108:VAL:HG22 | 2:D:469:PHE:HZ | 1.80 | 0.47 |
| 2:C:112:PHE:O | 2:C:115:TYR:HB3 | 2.14 | 0.47 |
| 2:C:189:TYR:O | 2:C:427:LYS:HE3 | 2.15 | 0.47 |
| 1:E:81:VAL:CG2 | 1:E:111:LEU:HD13 | 2.33 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:344:ARG:CG | 2:G:344:ARG:NH1 | 2.78 | 0.47 |
| 2:G:98:LEU:HD12 | 2:G:99:ASP:H | 1.80 | 0.47 |
| 2:H:549:ALA:O | 2:H:550:HIS:C | 2.52 | 0.47 |
| 1:A:168:ASP:H | 1:A:188:LEU:CD2 | 2.27 | 0.47 |
| 2:G:451:LEU:HD21 | 2:G:458:ARG:HG3 | 1.97 | 0.47 |
| 2:C:398:ILE:HG23 | 2:C:399:SER:N | 2.29 | 0.47 |
| 2:D:112:PHE:O | 2:D:115:TYR:HB3 | 2.15 | 0.47 |
| 2:H:373:GLU:O | 2:H:377:MET:HG3 | 2.15 | 0.47 |
| 2:D:173:TYR:HA | 2:D:176:GLU:HB2 | 1.95 | 0.47 |
| 1:F:193:ILE:CD1 | 1:F:245:ILE:HD13 | 2.44 | 0.47 |
| 2:G:457:TYR:CD1 | 2:G:457:TYR:C | 2.89 | 0.47 |
| 2:C:454:LEU:HD13 | 2:C:495:GLY:HA3 | 1.97 | 0.47 |
| 1:E:54:HIS:CE1 | 1:E:82:LYS:HB2 | 2.50 | 0.47 |
| 1:F:138:ASP:HA | 1:F:148:TRP:CE3 | 2.50 | 0.47 |
| 2:C:269:ASP:O | 2:C:270:LEU:O | 2.32 | 0.47 |
| 2:G:508:LEU:O | 2:G:510:HIS:N | 2.48 | 0.47 |
| 1:B:138:ASP:HA | 1:B:148:TRP:CE3 | 2.50 | 0.47 |
| 2:D:192:LEU:HD11 | 2:D:204:PHE:HD2 | 1.79 | 0.47 |
| 2:D:99:ASP:OD2 | 2:D:171:ARG:NE | 2.48 | 0.47 |
| 2:H:69:PHE:CD2 | 2:H:80:ALA:HB2 | 2.49 | 0.46 |
| 1:F:328:VAL:HG11 | 2:H:69:PHE:CG | 2.50 | 0.46 |
| 2:D:344:ARG:HH11 | 2:D:344:ARG:CG | 2.22 | 0.46 |
| 2:G:454:LEU:O | 2:G:454:LEU:HD12 | 2.15 | 0.46 |
| 1:A:324:ASP:HB3 | 2:C:64:LYS:HB3 | 1.96 | 0.46 |
| 1:E:168:ASP:H | 1:E:188:LEU:CD2 | 2.28 | 0.46 |
| 2:D:201:ARG:NH2 | 2:D:303:PHE:CD1 | 2.83 | 0.46 |
| 2:G:52:THR:HG22 | 2:G:54:ASN:H | 1.80 | 0.46 |
| 1:A:27:CYS:HB3 | 1:A:61:ILE:CD1 | 2.39 | 0.46 |
| 1:B:324:ASP:HB3 | 2:D:64:LYS:CG | 2.45 | 0.46 |
| 2:H:216:ASP:OD2 | 2:H:218:GLU:HB2 | 2.15 | 0.46 |
| 2:C:94:ARG:HH21 | 2:C:98:LEU:HB3 | 1.80 | 0.46 |
| 2:G:548:SER:HA | 2:G:551:ASN:ND2 | 2.30 | 0.46 |
| 2:H:112:PHE:O | 2:H:115:TYR:HB3 | 2.15 | 0.46 |
| 1:E:16:VAL:HG21 | 1:E:61:ILE:O | 2.15 | 0.46 |
| 2:C:344:ARG:NH1 | 2:C:344:ARG:HG3 | 2.24 | 0.46 |
| 2:H:271:LEU:N | 2:H:272:PRO:CD | 2.78 | 0.46 |
| 1:B:151:THR:CG2 | 1:B:196:ARG:HH22 | 2.29 | 0.46 |
| 2:H:86:ASP:HA | 2:H:88:TYR:HE1 | 1.79 | 0.46 |
| 2:G:272:PRO:O | 2:G:273:TYR:C | 2.53 | 0.46 |
| 2:C:526:CYS:O | 2:C:530:ARG:HA | 2.15 | 0.46 |
| 2:H:423:ILE:O | 2:H:426:ALA:HB3 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:86:GLU:HB2 | 1:E:98:TRP:CZ3 | 2.50 | 0.46 |
| 2:C:86:ASP:N | 2:C:88:TYR:CE1 | 2.82 | 0.46 |
| 1:F:169:PHE:O | 1:F:170:CYS:HB3 | 2.16 | 0.46 |
| 1:A:34:LYS:HE2 | 1:A:50:SER:OG | 2.14 | 0.46 |
| 1:F:97:ARG:HH11 | 1:F:97:ARG:HG3 | 1.80 | 0.46 |
| 2:C:552:ILE:O | 2:C:556:ILE:HG13 | 2.16 | 0.46 |
| 2:C:478:ASP:C | 2:C:480:GLU:N | 2.69 | 0.46 |
| 1:B:226:ARG:HG3 | 1:B:226:ARG:NH1 | 2.30 | 0.46 |
| 1:F:295:GLU:HG2 | 2:G:311:LEU:CD2 | 2.46 | 0.46 |
| 2:G:305:GLU:O | 2:G:309:LEU:HG | 2.15 | 0.46 |
| 2:C:460:GLY:C | 2:C:462:ALA:N | 2.69 | 0.46 |
| 1:F:302:ASP:OD2 | 2:H:44:SER:HB3 | 2.16 | 0.46 |
| 2:C:478:ASP:C | 2:C:480:GLU:H | 2.19 | 0.46 |
| 2:D:240:PHE:HD2 | 2:D:268:SER:CB | 2.29 | 0.46 |
| 2:C:457:TYR:C | 2:C:457:TYR:CD1 | 2.89 | 0.46 |
| 2:D:153:ASN:O | 2:D:156:GLU:N | 2.46 | 0.46 |
| 2:D:496:THR:HB | 2:D:499:ALA:H | 1.81 | 0.46 |
| 2:C:271:LEU:O | 2:C:275:SER:HB3 | 2.15 | 0.46 |
| 2:D:375:LEU:HD11 | 2:D:395:VAL:HG13 | 1.98 | 0.46 |
| 1:B:76:SER:OG | 1:B:77:TYR:N | 2.48 | 0.46 |
| 2:H:250:ASN:O | 2:H:254:LEU:HG | 2.16 | 0.46 |
| 1:F:125:LEU:C | 1:F:125:LEU:HD12 | 2.36 | 0.46 |
| 2:G:289:ILE:O | 2:G:293:LYS:HG3 | 2.15 | 0.46 |
| 2:D:184:CYS:HB2 | 2:D:211:TRP:CE2 | 2.50 | 0.46 |
| 2:C:269:ASP:O | 2:C:270:LEU:C | 2.53 | 0.46 |
| 2:G:423:ILE:O | 2:G:426:ALA:HB3 | 2.16 | 0.46 |
| 2:G:216:ASP:OD2 | 2:G:218:GLU:HB2 | 2.16 | 0.46 |
| 1:B:125:LEU:C | 1:B:125:LEU:HD12 | 2.36 | 0.46 |
| 1:E:125:LEU:C | 1:E:125:LEU:HD12 | 2.36 | 0.46 |
| 1:B:193:ILE:CD1 | 1:B:245:ILE:HD13 | 2.46 | 0.46 |
| 1:B:54:HIS:CE1 | 1:B:82:LYS:HB2 | 2.51 | 0.46 |
| 2:C:551:ASN:O | 2:C:554:GLU:N | 2.49 | 0.46 |
| 2:D:269:ASP:O | 2:D:270:LEU:O | 2.34 | 0.46 |
| 2:H:86:ASP:N | 2:H:88:TYR:CE1 | 2.82 | 0.46 |
| 2:G:352:THR:OG1 | 2:G:355:GLU:HG3 | 2.15 | 0.46 |
| 1:A:169:PHE:O | 1:A:170:CYS:HB3 | 2.16 | 0.46 |
| 1:B:48:SER:O | 1:B:49:ASP:HB2 | 2.15 | 0.46 |
| 2:C:43:VAL:CG1 | 2:C:48:LEU:CD2 | 2.79 | 0.46 |
| 1:E:208:LEU:HD11 | 1:E:231:ILE:HD12 | 1.96 | 0.46 |
| 2:H:344:ARG:CG | 2:H:344:ARG:NH1 | 2.78 | 0.46 |
| 1:A:54:HIS:CE1 | 1:A:82:LYS:HB2 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:138:ASP:HA | 1:E:148:TRP:CE3 | 2.51 | 0.46 |
| 1:E:309:SER:HB3 | 2:G:68:LYS:HA | 1.97 | 0.46 |
| 2:H:305:GLU:O | 2:H:309:LEU:HG | 2.16 | 0.46 |
| 1:E:136:LEU:HD11 | 1:E:202:LEU:HD11 | 1.97 | 0.46 |
| 2:D:343:GLN:HA | 2:D:360:PHE:HE1 | 1.80 | 0.46 |
| 2:C:480:GLU:O | 2:C:483:PRO:CD | 2.64 | 0.45 |
| 2:H:270:LEU:HD13 | 2:H:289:ILE:CD1 | 2.46 | 0.45 |
| 1:A:205:ALA:O | 1:A:206:ALA:HB2 | 2.15 | 0.45 |
| 1:B:79:LYS:HG2 | 1:B:110:SER:N | 2.31 | 0.45 |
| 2:D:117:ASP:C | 2:D:119:GLY:H | 2.19 | 0.45 |
| 2:G:171:ARG:O | 2:G:175:LEU:HG | 2.17 | 0.45 |
| 2:D:352:THR:OG1 | 2:D:355:GLU:HG3 | 2.16 | 0.45 |
| 1:F:208:LEU:HD11 | 1:F:231:ILE:HD12 | 1.96 | 0.45 |
| 1:A:16:VAL:HG21 | 1:A:61:ILE:O | 2.15 | 0.45 |
| 2:G:515:THR:CG2 | 2:G:516:ASN:H | 2.27 | 0.45 |
| 2:D:523:LEU:HD23 | 2:D:538:ILE:CD1 | 2.47 | 0.45 |
| 1:E:101:LEU:O | 1:E:102:CYS:HB2 | 2.16 | 0.45 |
| 2:G:104:PHE:O | 2:G:107:TYR:N | 2.49 | 0.45 |
| 2:C:459:ASN:N | 2:C:459:ASN:HD22 | 2.14 | 0.45 |
| 2:G:379:LEU:HD11 | 2:G:395:VAL:CG1 | 2.47 | 0.45 |
| 2:D:453:ASP:HB3 | 2:D:456:SER:HB2 | 1.97 | 0.45 |
| 2:G:308:ASN:HD22 | 2:G:308:ASN:C | 2.19 | 0.45 |
| 2:D:482:TRP:O | 2:D:485:ALA:HB3 | 2.16 | 0.45 |
| 2:H:352:THR:OG1 | 2:H:355:GLU:HG3 | 2.16 | 0.45 |
| 2:C:246:TRP:CE2 | 2:C:331:TYR:HB3 | 2.51 | 0.45 |
| 2:G:313:LEU:C | 2:G:313:LEU:HD23 | 2.36 | 0.45 |
| 1:A:326:GLY:CA | 2:C:58:ILE:HD12 | 2.44 | 0.45 |
| 1:F:205:ALA:O | 1:F:206:ALA:HB2 | 2.15 | 0.45 |
| 2:H:145:ASN:OD1 | 2:H:190:PHE:HA | 2.15 | 0.45 |
| 2:C:415:CYS:HB2 | 2:C:469:PHE:CE1 | 2.51 | 0.45 |
| 2:C:41:ASP:HA | 2:C:42:PRO:HD3 | 1.77 | 0.45 |
| 2:C:184:CYS:HB2 | 2:C:211:TRP:CE2 | 2.51 | 0.45 |
| 2:H:245:PHE:O | 2:H:248:LEU:HB3 | 2.17 | 0.45 |
| 2:C:145:ASN:OD1 | 2:C:190:PHE:HA | 2.16 | 0.45 |
| 1:A:151:THR:HG22 | 1:A:152:SER:N | 2.30 | 0.45 |
| 1:B:136:LEU:HD11 | 1:B:202:LEU:HD11 | 1.98 | 0.45 |
| 2:C:69:PHE:CE1 | 2:C:71:LEU:HD23 | 2.41 | 0.45 |
| 2:D:289:ILE:O | 2:D:293:LYS:HG3 | 2.17 | 0.45 |
| 2:H:531:LEU:HD13 | 2:H:534:ILE:CD1 | 2.46 | 0.45 |
| 2:G:153:ASN:O | 2:G:156:GLU:N | 2.46 | 0.45 |
| 2:D:263:GLY:O | 2:D:267:ARG:HG2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:114:VAL:HG23 | 1:F:126:ALA:O | 2.16 | 0.45 |
| 2:D:379:LEU:HD11 | 2:D:395:VAL:CG1 | 2.46 | 0.45 |
| 1:F:347:ALA:HB1 | 2:H:57:PRO:HG2 | 1.99 | 0.45 |
| 1:A:86:GLU:HB2 | 1:A:98:TRP:CZ3 | 2.52 | 0.45 |
| 1:E:74:SER:O | 1:E:81:VAL:HG13 | 2.17 | 0.45 |
| 1:F:137:TYR:HE1 | 1:F:150:LEU:HG | 1.80 | 0.45 |
| 1:B:54:HIS:HD2 | 1:B:58:ILE:HG12 | 1.81 | 0.45 |
| 2:H:81:PHE:HB3 | 2:H:90:LEU:HD23 | 1.99 | 0.45 |
| 2:H:523:LEU:O | 2:H:526:CYS:HB2 | 2.17 | 0.45 |
| 2:H:190:PHE:N | 2:H:190:PHE:CD1 | 2.85 | 0.45 |
| 2:D:250:ASN:O | 2:D:254:LEU:HG | 2.17 | 0.45 |
| 1:B:97:ARG:HH11 | 1:B:97:ARG:HG3 | 1.81 | 0.45 |
| 1:B:81:VAL:CG2 | 1:B:111:LEU:HD13 | 2.32 | 0.45 |
| 2:H:240:PHE:HD2 | 2:H:268:SER:CB | 2.29 | 0.45 |
| 2:H:289:ILE:O | 2:H:293:LYS:HG3 | 2.17 | 0.45 |
| 1:F:336:SER:HB2 | 2:G:343:GLN:OE1 | 2.17 | 0.45 |
| 2:D:204:PHE:CD1 | 2:D:205:ILE:N | 2.84 | 0.45 |
| 1:B:168:ASP:H | 1:B:188:LEU:CD2 | 2.29 | 0.45 |
| 2:C:163:LYS:CE | 2:C:168:ARG:HH21 | 2.29 | 0.45 |
| 1:A:1:MET:CE | 2:C:94:ARG:HD2 | 2.46 | 0.45 |
| 2:C:552:ILE:O | 2:C:556:ILE:N | 2.36 | 0.45 |
| 2:G:336:LEU:HA | 2:G:339:ILE:HD12 | 1.99 | 0.45 |
| 2:H:336:LEU:HA | 2:H:339:ILE:HD12 | 1.99 | 0.45 |
| 2:D:204:PHE:CD1 | 2:D:204:PHE:C | 2.90 | 0.45 |
| 2:C:204:PHE:CD1 | 2:C:204:PHE:C | 2.90 | 0.45 |
| 2:D:99:ASP:OD1 | 2:D:101:SER:HB2 | 2.17 | 0.45 |
| 1:E:151:THR:HG22 | 1:E:152:SER:N | 2.31 | 0.45 |
| 1:B:114:VAL:HG13 | 1:B:114:VAL:O | 2.17 | 0.45 |
| 2:C:216:ASP:OD2 | 2:C:218:GLU:HB2 | 2.16 | 0.45 |
| 1:E:47:LEU:HD12 | 1:E:48:SER:N | 2.32 | 0.45 |
| 2:D:492:SER:O | 2:D:494:THR:N | 2.50 | 0.45 |
| 2:G:269:ASP:O | 2:G:270:LEU:O | 2.35 | 0.45 |
| 2:C:153:ASN:O | 2:C:156:GLU:N | 2.48 | 0.45 |
| 2:C:98:LEU:HD12 | 2:C:99:ASP:H | 1.81 | 0.45 |
| 1:F:15:VAL:O | 2:H:70:LYS:HD2 | 2.17 | 0.45 |
| 2:H:482:TRP:N | 2:H:483:PRO:HD3 | 2.32 | 0.44 |
| 1:B:334:THR:CG2 | 1:B:335:TYR:H | 2.30 | 0.44 |
| 2:C:118:LEU:HD21 | 2:C:147:ALA:CB | 2.46 | 0.44 |
| 2:C:422:MET:SD | 2:C:423:ILE:N | 2.90 | 0.44 |
| 2:G:204:PHE:CD1 | 2:G:205:ILE:N | 2.84 | 0.44 |
| 2:H:118:LEU:O | 2:H:119:GLY:C | 2.56 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:183:LEU:HD12 | 1:F:184:ALA:H | 1.82 | 0.44 |
| 2:G:383:VAL:CG1 | 2:G:384:VAL:N | 2.80 | 0.44 |
| 2:C:190:PHE:N | 2:C:190:PHE:CD1 | 2.85 | 0.44 |
| 2:H:86:ASP:HA | 2:H:88:TYR:CE1 | 2.52 | 0.44 |
| 2:D:498:SER:O | 2:D:501:LYS:HB3 | 2.17 | 0.44 |
| 2:D:508:LEU:C | 2:D:510:HIS:H | 2.19 | 0.44 |
| 2:D:247:LYS:O | 2:D:251:GLN:HG3 | 2.18 | 0.44 |
| 2:G:396:ASP:OD1 | 2:G:401:LYS:HE3 | 2.16 | 0.44 |
| 1:A:334:THR:CG2 | 1:A:335:TYR:H | 2.30 | 0.44 |
| 2:C:118:LEU:O | 2:C:119:GLY:C | 2.55 | 0.44 |
| 2:G:204:PHE:CD1 | 2:G:204:PHE:C | 2.90 | 0.44 |
| 2:H:524:SER:O | 2:H:527:VAL:N | 2.50 | 0.44 |
| 2:C:126:VAL:HG12 | 2:C:126:VAL:O | 2.16 | 0.44 |
| 1:E:97:ARG:HG3 | 1:E:97:ARG:HH11 | 1.81 | 0.44 |
| 2:H:269:ASP:O | 2:H:270:LEU:O | 2.35 | 0.44 |
| 2:C:240:PHE:HD2 | 2:C:268:SER:CB | 2.29 | 0.44 |
| 2:C:523:LEU:CD2 | 2:C:538:ILE:CD1 | 2.95 | 0.44 |
| 2:C:104:PHE:C | 2:C:106:ALA:H | 2.20 | 0.44 |
| 2:G:189:TYR:O | 2:G:427:LYS:HE3 | 2.17 | 0.44 |
| 2:D:305:GLU:O | 2:D:309:LEU:HG | 2.17 | 0.44 |
| 2:H:179:LEU:O | 2:H:182:LEU:N | 2.50 | 0.44 |
| 2:C:179:LEU:O | 2:C:182:LEU:N | 2.50 | 0.44 |
| 1:E:334:THR:CG2 | 1:E:335:TYR:H | 2.29 | 0.44 |
| 2:H:117:ASP:C | 2:H:119:GLY:H | 2.20 | 0.44 |
| 2:H:531:LEU:CD1 | 2:H:534:ILE:HD12 | 2.48 | 0.44 |
| 2:H:471:PHE:C | 2:H:473:LEU:N | 2.71 | 0.44 |
| 1:E:151:THR:CG2 | 1:E:196:ARG:HH22 | 2.31 | 0.44 |
| 2:D:189:TYR:O | 2:D:427:LYS:HE3 | 2.16 | 0.44 |
| 2:H:343:GLN:HA | 2:H:360:PHE:HE1 | 1.82 | 0.44 |
| 2:D:271:LEU:O | 2:D:275:SER:HB3 | 2.18 | 0.44 |
| 2:D:373:GLU:O | 2:D:377:MET:HG3 | 2.17 | 0.44 |
| 1:E:224:ILE:HG22 | 2:G:503:VAL:HG13 | 1.99 | 0.44 |
| 1:B:309:SER:HB3 | 2:D:68:LYS:HA | 1.99 | 0.44 |
| 1:E:76:SER:OG | 1:E:77:TYR:N | 2.50 | 0.44 |
| 1:F:171:LEU:HB3 | 1:F:185:VAL:HG13 | 1.99 | 0.44 |
| 2:G:235:ALA:O | 2:G:237:LYS:N | 2.48 | 0.44 |
| 1:E:48:SER:O | 1:E:49:ASP:HB2 | 2.17 | 0.44 |
| 2:C:352:THR:OG1 | 2:C:355:GLU:HG3 | 2.18 | 0.44 |
| 2:C:42:PRO:CB | 2:C:46:ALA:O | 2.66 | 0.44 |
| 2:C:47:ILE:HG22 | 2:C:48:LEU:N | 2.33 | 0.44 |
| 1:B:16:VAL:HG21 | 1:B:61:ILE:O | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:137:TYR:HE1 | 1:E:150:LEU:HG | 1.81 | 0.44 |
| 2:H:555:SER:CA | 2:H:558:ASN:HB3 | 2.46 | 0.44 |
| 2:H:104:PHE:C | 2:H:106:ALA:H | 2.19 | 0.44 |
| 2:G:145:ASN:OD1 | 2:G:190:PHE:HA | 2.18 | 0.44 |
| 2:C:456:SER:OG | 2:C:457:TYR:N | 2.51 | 0.44 |
| 2:C:305:GLU:O | 2:C:308:ASN:HB3 | 2.17 | 0.44 |
| 2:C:247:LYS:O | 2:C:251:GLN:HG3 | 2.18 | 0.44 |
| 2:H:214:ARG:O | 2:H:214:ARG:HG3 | 2.17 | 0.44 |
| 2:C:214:ARG:HG3 | 2:C:214:ARG:O | 2.17 | 0.44 |
| 2:C:344:ARG:CG | 2:C:344:ARG:NH1 | 2.77 | 0.44 |
| 1:E:315:THR:HB | 2:G:471:PHE:HD2 | 1.82 | 0.44 |
| 1:F:309:SER:HB3 | 2:H:68:LYS:HA | 1.99 | 0.44 |
| 2:G:508:LEU:C | 2:G:510:HIS:N | 2.71 | 0.44 |
| 1:E:205:ALA:O | 1:E:206:ALA:HB2 | 2.18 | 0.44 |
| 2:H:523:LEU:HD23 | 2:H:538:ILE:HD12 | 2.00 | 0.44 |
| 2:D:525:ILE:C | 2:D:527:VAL:N | 2.71 | 0.44 |
| 2:C:171:ARG:O | 2:C:175:LEU:HG | 2.18 | 0.44 |
| 2:C:551:ASN:O | 2:C:554:GLU:CB | 2.65 | 0.44 |
| 2:G:343:GLN:HA | 2:G:360:PHE:HE1 | 1.82 | 0.44 |
| 1:A:124:LYS:HA | 1:A:138:ASP:HB3 | 1.99 | 0.44 |
| 2:G:190:PHE:CD1 | 2:G:190:PHE:N | 2.85 | 0.44 |
| 1:F:228:TYR:CD2 | 1:F:244:LYS:HG3 | 2.52 | 0.44 |
| 2:H:163:LYS:CE | 2:H:168:ARG:HH21 | 2.30 | 0.44 |
| 2:G:163:LYS:CE | 2:G:168:ARG:HH21 | 2.31 | 0.44 |
| 2:G:103:GLU:N | 2:G:103:GLU:CD | 2.71 | 0.44 |
| 1:B:86:GLU:HB2 | 1:B:98:TRP:CZ3 | 2.52 | 0.44 |
| 1:B:114:VAL:HG23 | 1:B:126:ALA:O | 2.17 | 0.44 |
| 2:C:343:GLN:HA | 2:C:360:PHE:HE1 | 1.82 | 0.44 |
| 1:A:125:LEU:HD12 | 1:A:125:LEU:C | 2.38 | 0.44 |
| 2:H:274:LEU:HD22 | 2:H:281:SER:CB | 2.47 | 0.44 |
| 1:F:334:THR:CG2 | 1:F:335:TYR:H | 2.29 | 0.44 |
| 2:D:270:LEU:HD13 | 2:D:289:ILE:CD1 | 2.48 | 0.44 |
| 2:C:81:PHE:HB3 | 2:C:90:LEU:HD23 | 2.00 | 0.44 |
| 1:E:15:VAL:HB | 2:G:81:PHE:CE2 | 2.53 | 0.44 |
| 2:D:171:ARG:O | 2:D:175:LEU:HG | 2.18 | 0.44 |
| 1:A:108:LYS:HE2 | 1:A:133:ILE:HD12 | 2.00 | 0.44 |
| 2:H:85:LYS:O | 2:H:86:ASP:HB2 | 2.18 | 0.44 |
| 1:B:47:LEU:HD12 | 1:B:48:SER:N | 2.32 | 0.44 |
| 2:H:246:TRP:CE2 | 2:H:331:TYR:HB3 | 2.53 | 0.44 |
| 2:D:216:ASP:OD2 | 2:D:218:GLU:HB2 | 2.18 | 0.44 |
| 1:A:59:VAL:HG12 | 1:A:59:VAL:O | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:137:TYR:HE1 | 1:B:150:LEU:HG | 1.82 | 0.43 |
| 2:D:336:LEU:HA | 2:D:339:ILE:HD12 | 1.99 | 0.43 |
| 1:A:137:TYR:HE1 | 1:A:150:LEU:HG | 1.82 | 0.43 |
| 2:H:258:LEU:HD22 | 2:H:292:LEU:CD2 | 2.44 | 0.43 |
| 1:E:54:HIS:CD2 | 1:E:58:ILE:HG12 | 2.53 | 0.43 |
| 2:H:486:ILE:O | 2:H:490:ALA:HB2 | 2.18 | 0.43 |
| 2:C:289:ILE:O | 2:C:293:LYS:HG3 | 2.17 | 0.43 |
| 1:F:345:ILE:HA | 2:H:49:VAL:O | 2.18 | 0.43 |
| 2:H:541:THR:HG22 | 2:H:545:GLN:NE2 | 2.33 | 0.43 |
| 2:C:204:PHE:O | 2:C:207:SER:N | 2.51 | 0.43 |
| 1:B:15:VAL:HG21 | 2:D:90:LEU:HD21 | 2.00 | 0.43 |
| 1:B:1:MET:CE | 2:D:94:ARG:HD2 | 2.47 | 0.43 |
| 1:B:205:ALA:O | 1:B:206:ALA:HB2 | 2.17 | 0.43 |
| 2:H:470:ALA:HB1 | 2:H:489:ILE:HG13 | 2.00 | 0.43 |
| 1:E:79:LYS:HG2 | 1:E:110:SER:N | 2.33 | 0.43 |
| 2:D:104:PHE:C | 2:D:106:ALA:N | 2.72 | 0.43 |
| 1:F:310:VAL:HA | 1:F:320:SER:O | 2.17 | 0.43 |
| 1:B:74:SER:O | 1:B:81:VAL:HG13 | 2.18 | 0.43 |
| 1:E:10:ASP:C | 2:G:88:TYR:CE2 | 2.90 | 0.43 |
| 2:D:69:PHE:CD2 | 2:D:80:ALA:HB2 | 2.53 | 0.43 |
| 2:D:197:VAL:CB | 2:D:366:PRO:HB2 | 2.48 | 0.43 |
| 2:H:415:CYS:HB2 | 2:H:469:PHE:CE1 | 2.51 | 0.43 |
| 1:F:170:CYS:SG | 1:F:218:ILE:HG22 | 2.59 | 0.43 |
| 1:E:6:SER:HB2 | 1:E:8:HIS:HD2 | 1.84 | 0.43 |
| 2:C:250:ASN:O | 2:C:254:LEU:HG | 2.17 | 0.43 |
| 1:B:28:SER:OG | 1:B:30:ASP:OD1 | 2.36 | 0.43 |
| 2:H:481:LEU:O | 2:H:484:VAL:HB | 2.19 | 0.43 |
| 1:E:314:LEU:CD2 | 2:G:73:PRO:O | 2.67 | 0.43 |
| 1:B:59:VAL:O | 1:B:59:VAL:HG12 | 2.18 | 0.43 |
| 2:C:515:THR:CG2 | 2:C:516:ASN:H | 2.31 | 0.43 |
| 1:A:25:ALA:O | 1:A:61:ILE:HD12 | 2.18 | 0.43 |
| 1:E:328:VAL:HG11 | 2:G:69:PHE:CG | 2.53 | 0.43 |
| 1:B:145:LEU:N | 1:B:145:LEU:HD12 | 2.33 | 0.43 |
| 2:H:526:CYS:O | 2:H:530:ARG:N | 2.47 | 0.43 |
| 1:B:169:PHE:O | 1:B:170:CYS:HB3 | 2.19 | 0.43 |
| 2:D:344:ARG:CG | 2:D:344:ARG:NH1 | 2.79 | 0.43 |
| 2:H:269:ASP:O | 2:H:270:LEU:C | 2.55 | 0.43 |
| 2:G:184:CYS:HB2 | 2:G:211:TRP:CE2 | 2.54 | 0.43 |
| 2:D:163:LYS:CE | 2:D:168:ARG:HH21 | 2.29 | 0.43 |
| 1:A:170:CYS:SG | 1:A:218:ILE:HG22 | 2.59 | 0.43 |
| 2:G:253:VAL:HG21 | 2:G:335:PHE:CE1 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:274:LEU:HD22 | 2:G:281:SER:CB | 2.47 | 0.43 |
| 2:H:478:ASP:O | 2:H:480:GLU:N | 2.51 | 0.43 |
| 2:G:198:GLU:HA | 2:G:300:SER:OG | 2.17 | 0.43 |
| 1:F:101:LEU:O | 1:F:102:CYS:HB2 | 2.17 | 0.43 |
| 2:D:81:PHE:HB3 | 2:D:90:LEU:HD23 | 2.00 | 0.43 |
| 2:D:197:VAL:HB | 2:D:366:PRO:O | 2.19 | 0.43 |
| 2:G:104:PHE:C | 2:G:106:ALA:H | 2.21 | 0.43 |
| 2:G:151:ILE:O | 2:G:152:LEU:C | 2.57 | 0.43 |
| 2:D:492:SER:C | 2:D:494:THR:H | 2.22 | 0.43 |
| 1:E:199:ASP:OD2 | 1:E:201:LYS:HB2 | 2.18 | 0.43 |
| 1:A:47:LEU:HD12 | 1:A:48:SER:N | 2.34 | 0.43 |
| 2:G:263:GLY:O | 2:G:267:ARG:HG2 | 2.19 | 0.43 |
| 2:G:40:ARG:O | 2:G:42:PRO:HD3 | 2.19 | 0.43 |
| 2:C:482:TRP:O | 2:C:486:ILE:HG12 | 2.19 | 0.43 |
| 2:D:85:LYS:O | 2:D:86:ASP:HB2 | 2.18 | 0.43 |
| 1:E:117:ALA:HB2 | 1:E:173:TRP:CE2 | 2.53 | 0.43 |
| 2:C:167:GLY:O | 2:C:168:ARG:HG3 | 2.18 | 0.43 |
| 2:C:527:VAL:HG12 | 2:C:528:GLU:N | 2.34 | 0.43 |
| 2:D:108:VAL:HG12 | 2:D:484:VAL:HG11 | 2.01 | 0.43 |
| 2:H:555:SER:HA | 2:H:558:ASN:OD1 | 2.19 | 0.43 |
| 1:A:76:SER:OG | 1:A:77:TYR:N | 2.51 | 0.43 |
| 2:C:226:GLN:C | 2:C:228:PHE:H | 2.21 | 0.43 |
| 1:F:6:SER:HB2 | 1:F:8:HIS:HD2 | 1.84 | 0.43 |
| 2:D:253:VAL:HG21 | 2:D:335:PHE:CE1 | 2.53 | 0.43 |
| 2:C:258:LEU:HD22 | 2:C:292:LEU:CD2 | 2.42 | 0.43 |
| 2:G:99:ASP:OD1 | 2:G:101:SER:HB2 | 2.18 | 0.43 |
| 2:C:117:ASP:C | 2:C:119:GLY:H | 2.22 | 0.43 |
| 2:G:81:PHE:HB3 | 2:G:90:LEU:HD23 | 2.00 | 0.43 |
| 2:H:197:VAL:HB | 2:H:366:PRO:HB2 | 2.01 | 0.43 |
| 1:E:169:PHE:O | 1:E:170:CYS:HB3 | 2.19 | 0.43 |
| 2:H:459:ASN:OD1 | 2:H:494:THR:HB | 2.18 | 0.43 |
| 2:D:515:THR:HB | 2:D:518:ASP:OD1 | 2.18 | 0.43 |
| 1:A:328:VAL:HG11 | 2:C:69:PHE:CG | 2.54 | 0.43 |
| 1:B:11:LEU:N | 2:D:88:TYR:HE2 | 2.17 | 0.43 |
| 2:G:508:LEU:HB3 | 2:G:534:ILE:HD13 | 2.01 | 0.43 |
| 2:H:89:LYS:HD2 | 2:H:89:LYS:H | 1.82 | 0.43 |
| 2:H:201:ARG:NH1 | 2:H:201:ARG:HG3 | 2.33 | 0.43 |
| 2:G:67:LEU:HD12 | 2:G:81:PHE:O | 2.19 | 0.43 |
| 2:H:305:GLU:O | 2:H:308:ASN:HB3 | 2.19 | 0.43 |
| 2:H:226:GLN:C | 2:H:228:PHE:H | 2.22 | 0.43 |
| 2:G:247:LYS:O | 2:G:251:GLN:HG3 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:G:460:GLY:O | 2:G:463:SER:N | 2.52 | 0.43 |
| 2:D:533:GLU:OE1 | 2:D:533:GLU:HA | 2.19 | 0.43 |
| 2:G:519:ILE:O | 2:G:523:LEU:HG | 2.19 | 0.42 |
| 2:H:553:ILE:O | 2:H:556:ILE:CG2 | 2.67 | 0.42 |
| 2:C:406:LEU:HB2 | 2:C:407:PRO:CD | 2.44 | 0.42 |
| 2:G:271:LEU:O | 2:G:275:SER:HB3 | 2.19 | 0.42 |
| 2:C:270:LEU:HD13 | 2:C:289:ILE:CD1 | 2.49 | 0.42 |
| 2:G:94:ARG:HH21 | 2:G:98:LEU:HB3 | 1.83 | 0.42 |
| 2:H:81:PHE:C | 2:H:81:PHE:CD1 | 2.92 | 0.42 |
| 1:A:303:HIS:HD1 | 1:A:325:ASP:CG | 2.22 | 0.42 |
| 2:C:104:PHE:O | 2:C:107:TYR:N | 2.51 | 0.42 |
| 2:D:383:VAL:CG1 | 2:D:384:VAL:N | 2.81 | 0.42 |
| 2:D:226:GLN:C | 2:D:228:PHE:H | 2.21 | 0.42 |
| 1:F:314:LEU:HD21 | 2:H:475:SER:OG | 2.19 | 0.42 |
| 1:A:82:LYS:HE3 | 1:A:100:LYS:HD3 | 2.00 | 0.42 |
| 2:H:480:GLU:O | 2:H:483:PRO:CD | 2.66 | 0.42 |
| 2:C:252:LEU:HD23 | 2:C:252:LEU:HA | 1.89 | 0.42 |
| 2:H:204:PHE:O | 2:H:207:SER:N | 2.52 | 0.42 |
| 2:G:197:VAL:HB | 2:G:366:PRO:O | 2.19 | 0.42 |
| 2:C:529:TRP:O | 2:C:530:ARG:HB2 | 2.18 | 0.42 |
| 1:F:86:GLU:HB2 | 1:F:98:TRP:CZ3 | 2.54 | 0.42 |
| 2:G:460:GLY:C | 2:G:462:ALA:N | 2.72 | 0.42 |
| 2:C:89:LYS:H | 2:C:89:LYS:HD2 | 1.80 | 0.42 |
| 1:E:114:VAL:HG13 | 1:E:114:VAL:O | 2.19 | 0.42 |
| 2:H:231:LYS:CG | 2:H:232:ASP:H | 2.29 | 0.42 |
| 1:F:27:CYS:HB3 | 1:F:61:ILE:CD1 | 2.40 | 0.42 |
| 2:G:85:LYS:O | 2:G:86:ASP:HB2 | 2.18 | 0.42 |
| 2:D:324:ILE:O | 2:D:325:SER:C | 2.58 | 0.42 |
| 2:C:204:PHE:CD1 | 2:C:205:ILE:N | 2.87 | 0.42 |
| 1:E:183:LEU:HD12 | 1:E:184:ALA:H | 1.85 | 0.42 |
| 1:B:314:LEU:CD2 | 2:D:73:PRO:O | 2.67 | 0.42 |
| 2:D:86:ASP:CA | 2:D:88:TYR:CE1 | 3.03 | 0.42 |
| 2:H:204:PHE:CD1 | 2:H:204:PHE:C | 2.92 | 0.42 |
| 2:H:526:CYS:O | 2:H:530:ARG:HA | 2.20 | 0.42 |
| 2:H:104:PHE:C | 2:H:106:ALA:N | 2.72 | 0.42 |
| 1:B:151:THR:HG22 | 1:B:152:SER:N | 2.32 | 0.42 |
| 2:C:305:GLU:O | 2:C:309:LEU:HG | 2.20 | 0.42 |
| 2:D:202:SER:HA | 2:D:297:LYS:O | 2.19 | 0.42 |
| 1:A:199:ASP:OD2 | 1:A:201:LYS:HD2 | 2.19 | 0.42 |
| 2:D:238:LYS:O | 2:D:239:VAL:C | 2.57 | 0.42 |
| 1:B:22:ARG:HA | 1:B:22:ARG:HD3 | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:27:CYS:SG | 1:B:27:CYS:O | 2.78 | 0.42 |
| 1:E:28:SER:OG | 1:E:30:ASP:OD1 | 2.37 | 0.42 |
| 2:D:69:PHE:HD2 | 2:D:80:ALA:HB2 | 1.83 | 0.42 |
| 1:F:156:VAL:HG12 | 1:F:157:LEU:N | 2.34 | 0.42 |
| 2:D:498:SER:O | 2:D:499:ALA:C | 2.57 | 0.42 |
| 2:D:179:LEU:O | 2:D:182:LEU:N | 2.52 | 0.42 |
| 2:H:42:PRO:HD2 | 2:H:46:ALA:O | 2.19 | 0.42 |
| 2:C:336:LEU:HA | 2:C:339:ILE:HD12 | 2.00 | 0.42 |
| 2:H:551:ASN:O | 2:H:555:SER:HB2 | 2.20 | 0.42 |
| 1:B:101:LEU:O | 1:B:102:CYS:HB2 | 2.18 | 0.42 |
| 2:D:89:LYS:H | 2:D:89:LYS:HD2 | 1.82 | 0.42 |
| 2:D:94:ARG:HH21 | 2:D:98:LEU:HB3 | 1.83 | 0.42 |
| 2:H:459:ASN:HB3 | 2:H:494:THR:HB | 2.02 | 0.42 |
| 2:G:145:ASN:O | 2:G:148:MET:HB3 | 2.20 | 0.42 |
| 2:D:112:PHE:CE1 | 2:D:488:LEU:HD13 | 2.54 | 0.42 |
| 2:C:103:GLU:N | 2:C:103:GLU:CD | 2.73 | 0.42 |
| 1:A:199:ASP:OD2 | 1:A:201:LYS:HB2 | 2.20 | 0.42 |
| 2:C:487:GLY:O | 2:C:488:LEU:C | 2.57 | 0.42 |
| 1:F:80:THR:HG22 | 1:F:105:ASN:HA | 2.01 | 0.42 |
| 1:F:199:ASP:OD2 | 1:F:201:LYS:HD2 | 2.19 | 0.42 |
| 1:E:59:VAL:O | 1:E:59:VAL:HG12 | 2.19 | 0.42 |
| 1:A:22:ARG:HD3 | 1:A:22:ARG:HA | 1.85 | 0.42 |
| 1:B:328:VAL:HG11 | 2:D:69:PHE:CG | 2.55 | 0.42 |
| 1:F:116:PHE:HD1 | 1:F:124:LYS:O | 2.03 | 0.42 |
| 1:B:117:ALA:HB2 | 1:B:173:TRP:CE2 | 2.55 | 0.42 |
| 2:H:103:GLU:CD | 2:H:103:GLU:N | 2.73 | 0.42 |
| 1:B:178:PHE:CE2 | 2:D:502:MET:HG2 | 2.55 | 0.42 |
| 2:D:396:ASP:OD1 | 2:D:401:LYS:HE3 | 2.19 | 0.42 |
| 1:F:245:ILE:HA | 1:F:293:GLN:O | 2.20 | 0.42 |
| 2:G:270:LEU:HD13 | 2:G:289:ILE:CD1 | 2.49 | 0.42 |
| 1:E:82:LYS:HE3 | 1:E:100:LYS:HD3 | 2.02 | 0.42 |
| 2:G:204:PHE:O | 2:G:207:SER:N | 2.53 | 0.42 |
| 2:D:167:GLY:O | 2:D:168:ARG:HG3 | 2.20 | 0.42 |
| 1:A:91:GLU:O | 1:A:97:ARG:HD2 | 2.20 | 0.42 |
| 2:G:218:GLU:HA | 2:G:220:ASP:N | 2.35 | 0.42 |
| 2:H:342:ASN:O | 2:H:343:GLN:C | 2.58 | 0.42 |
| 1:B:80:THR:HG22 | 1:B:105:ASN:HA | 2.02 | 0.42 |
| 1:B:320:SER:HB3 | 2:D:71:LEU:HD21 | 2.02 | 0.42 |
| 2:G:69:PHE:CE1 | 2:G:71:LEU:HD23 | 2.45 | 0.42 |
| 2:G:373:GLU:O | 2:G:377:MET:HG3 | 2.20 | 0.42 |
| 2:C:274:LEU:HD22 | 2:C:281:SER:CB | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:196:ASP:C | 2:C:198:GLU:N | 2.73 | 0.42 |
| 2:G:547:LEU:C | 2:G:549:ALA:N | 2.73 | 0.42 |
| 1:A:114:VAL:HG13 | 1:A:114:VAL:O | 2.20 | 0.42 |
| 1:A:310:VAL:HA | 1:A:320:SER:O | 2.20 | 0.42 |
| 2:D:492:SER:C | 2:D:494:THR:N | 2.74 | 0.42 |
| 1:E:114:VAL:HG23 | 1:E:126:ALA:O | 2.19 | 0.42 |
| 2:D:365:ILE:HB | 2:D:374:TYR:OH | 2.20 | 0.42 |
| 1:A:313:ASN:HB3 | 1:A:317:THR:H | 1.84 | 0.42 |
| 1:E:61:ILE:HG22 | 1:E:62:ASP:N | 2.35 | 0.41 |
| 1:F:16:VAL:HG21 | 1:F:61:ILE:O | 2.19 | 0.41 |
| 2:D:258:LEU:HD22 | 2:D:292:LEU:CD2 | 2.42 | 0.41 |
| 1:A:54:HIS:HD2 | 1:A:58:ILE:HG12 | 1.85 | 0.41 |
| 2:G:508:LEU:C | 2:G:510:HIS:H | 2.23 | 0.41 |
| 1:E:124:LYS:HA | 1:E:138:ASP:HB3 | 2.01 | 0.41 |
| 2:H:457:TYR:CD1 | 2:H:457:TYR:C | 2.93 | 0.41 |
| 1:A:117:ALA:HB2 | 1:A:173:TRP:CE2 | 2.55 | 0.41 |
| 2:H:467:ASN:OD1 | 2:H:467:ASN:N | 2.51 | 0.41 |
| 2:G:357:PHE:CE1 | 2:G:398:ILE:HD11 | 2.56 | 0.41 |
| 1:E:23:HIS:HD2 | 1:E:37:LYS:HA | 1.84 | 0.41 |
| 1:B:199:ASP:OD2 | 1:B:201:LYS:HB2 | 2.20 | 0.41 |
| 1:B:208:LEU:HD11 | 1:B:231:ILE:HD12 | 1.99 | 0.41 |
| 1:E:1:MET:CE | 2:G:94:ARG:HD2 | 2.49 | 0.41 |
| 2:C:81:PHE:CD1 | 2:C:81:PHE:C | 2.93 | 0.41 |
| 1:A:101:LEU:O | 1:A:102:CYS:HB2 | 2.19 | 0.41 |
| 2:G:197:VAL:CB | 2:G:366:PRO:HB2 | 2.50 | 0.41 |
| 2:H:469:PHE:O | 2:H:470:ALA:C | 2.58 | 0.41 |
| 2:C:383:VAL:CG1 | 2:C:384:VAL:N | 2.81 | 0.41 |
| 2:D:103:GLU:N | 2:D:103:GLU:CD | 2.73 | 0.41 |
| 2:G:226:GLN:C | 2:G:228:PHE:H | 2.23 | 0.41 |
| 2:D:83:THR:O | 2:D:84:ALA:HB2 | 2.20 | 0.41 |
| 2:G:473:LEU:HB2 | 2:G:485:ALA:HB2 | 2.02 | 0.41 |
| 2:C:231:LYS:NZ | 2:C:233:SER:HB3 | 2.35 | 0.41 |
| 2:H:253:VAL:HG21 | 2:H:335:PHE:CE1 | 2.55 | 0.41 |
| 2:G:201:ARG:NH2 | 2:G:303:PHE:CD1 | 2.88 | 0.41 |
| 2:H:200:ASN:O | 2:H:201:ARG:C | 2.59 | 0.41 |
| 2:D:248:LEU:O | 2:D:248:LEU:HD23 | 2.20 | 0.41 |
| 1:F:206:ALA:HB1 | 2:G:315:GLN:OE1 | 2.20 | 0.41 |
| 1:F:247:GLU:O | 1:F:247:GLU:HG3 | 2.20 | 0.41 |
| 1:A:48:SER:O | 1:A:49:ASP:HB2 | 2.20 | 0.41 |
| 2:C:228:PHE:CE2 | 2:C:267:ARG:HG3 | 2.55 | 0.41 |
| 1:F:47:LEU:HD12 | 1:F:48:SER:N | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:171:ARG:O | 2:H:175:LEU:HG | 2.20 | 0.41 |
| 2:D:142:ALA:O | 2:D:146:LEU:HG | 2.21 | 0.41 |
| 2:D:511:TYR:HA | 2:D:512:PRO:HD3 | 1.81 | 0.41 |
| 2:H:557:ALA:O | 2:H:561:ARG:N | 2.40 | 0.41 |
| 2:G:83:THR:O | 2:G:84:ALA:HB2 | 2.20 | 0.41 |
| 2:G:491:LEU:O | 2:G:493:ALA:N | 2.54 | 0.41 |
| 1:F:124:LYS:HA | 1:F:138:ASP:HB3 | 2.01 | 0.41 |
| 1:A:347:ALA:HB1 | 2:C:57:PRO:HG2 | 2.03 | 0.41 |
| 1:B:124:LYS:HA | 1:B:138:ASP:HB3 | 2.02 | 0.41 |
| 2:H:201:ARG:HH11 | 2:H:201:ARG:HG3 | 1.85 | 0.41 |
| 1:A:171:LEU:HB3 | 1:A:185:VAL:HG13 | 2.01 | 0.41 |
| 1:E:156:VAL:HG12 | 1:E:157:LEU:N | 2.36 | 0.41 |
| 2:C:167:GLY:O | 2:C:168:ARG:CG | 2.68 | 0.41 |
| 1:E:242:ILE:HD11 | 1:E:319:LEU:CD2 | 2.50 | 0.41 |
| 2:D:305:GLU:O | 2:D:308:ASN:HB3 | 2.20 | 0.41 |
| 2:C:407:PRO:O | 2:C:410:GLU:HB3 | 2.21 | 0.41 |
| 2:D:204:PHE:O | 2:D:207:SER:N | 2.53 | 0.41 |
| 2:C:104:PHE:C | 2:C:106:ALA:N | 2.73 | 0.41 |
| 1:B:303:HIS:HD1 | 1:B:325:ASP:CG | 2.24 | 0.41 |
| 1:A:226:ARG:HG3 | 1:A:226:ARG:NH1 | 2.34 | 0.41 |
| 2:C:173:TYR:HD1 | 2:C:173:TYR:H | 1.68 | 0.41 |
| 1:E:199:ASP:OD2 | 1:E:201:LYS:HD2 | 2.20 | 0.41 |
| 2:G:228:PHE:CE2 | 2:G:267:ARG:HG3 | 2.56 | 0.41 |
| 1:F:199:ASP:OD2 | 1:F:201:LYS:HB2 | 2.20 | 0.41 |
| 1:A:21:GLY:HA3 | 2:C:73:PRO:HD2 | 2.02 | 0.41 |
| 2:H:263:GLY:O | 2:H:267:ARG:HG2 | 2.19 | 0.41 |
| 1:A:81:VAL:CG2 | 1:A:111:LEU:HD13 | 2.36 | 0.41 |
| 2:C:550:HIS:HA | 2:C:553:ILE:CG1 | 2.50 | 0.41 |
| 1:F:54:HIS:HE1 | 1:F:82:LYS:HB2 | 1.85 | 0.41 |
| 2:C:296:PRO:HD3 | 2:C:306:TRP:CD1 | 2.55 | 0.41 |
| 2:H:532:PRO:O | 2:H:536:LYS:HG3 | 2.21 | 0.41 |
| 1:E:54:HIS:HE1 | 1:E:82:LYS:HB2 | 1.85 | 0.41 |
| 2:D:57:PRO:HG2 | 2:D:58:ILE:H | 1.86 | 0.41 |
| 2:G:375:LEU:HD11 | 2:G:395:VAL:HG13 | 2.01 | 0.41 |
| 2:H:383:VAL:CG1 | 2:H:384:VAL:N | 2.83 | 0.41 |
| 2:D:190:PHE:CE2 | 2:D:427:LYS:HG3 | 2.56 | 0.41 |
| 2:C:461:MET:O | 2:C:465:MET:HG3 | 2.21 | 0.41 |
| 1:B:23:HIS:HD2 | 1:B:37:LYS:HA | 1.85 | 0.41 |
| 2:H:478:ASP:C | 2:H:480:GLU:N | 2.74 | 0.41 |
| 2:C:245:PHE:O | 2:C:248:LEU:HB3 | 2.20 | 0.41 |
| 1:E:117:ALA:HA | 1:E:173:TRP:CG | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:190:PHE:N | 2:D:190:PHE:CD1 | 2.87 | 0.41 |
| 2:D:313:LEU:O | 2:D:313:LEU:HD23 | 2.19 | 0.41 |
| 2:G:142:ALA:O | 2:G:146:LEU:HG | 2.21 | 0.41 |
| 2:G:456:SER:OG | 2:G:457:TYR:N | 2.54 | 0.41 |
| 2:G:516:ASN:HA | 2:G:519:ILE:HD12 | 2.01 | 0.41 |
| 2:D:466:LEU:HA | 2:D:466:LEU:HD23 | 1.92 | 0.41 |
| 2:G:253:VAL:HG21 | 2:G:335:PHE:HE1 | 1.85 | 0.41 |
| 1:B:54:HIS:HE1 | 1:B:82:LYS:HB2 | 1.86 | 0.41 |
| 2:C:511:TYR:CE2 | 2:C:513:PHE:HB3 | 2.56 | 0.41 |
| 2:C:205:ILE:O | 2:C:205:ILE:HG22 | 2.20 | 0.41 |
| 2:G:104:PHE:C | 2:G:106:ALA:N | 2.74 | 0.41 |
| 1:B:156:VAL:HG12 | 1:B:157:LEU:N | 2.35 | 0.41 |
| 1:E:221:ALA:HA | 1:E:222:PRO:HD3 | 1.87 | 0.41 |
| 2:H:99:ASP:OD1 | 2:H:101:SER:HB2 | 2.20 | 0.41 |
| 2:H:173:TYR:HD1 | 2:H:173:TYR:H | 1.69 | 0.41 |
| 2:G:347:LEU:O | 2:G:348:GLN:C | 2.57 | 0.41 |
| 2:H:313:LEU:HD23 | 2:H:313:LEU:C | 2.41 | 0.41 |
| 1:F:25:ALA:O | 1:F:61:ILE:HD12 | 2.20 | 0.41 |
| 2:G:296:PRO:HD3 | 2:G:306:TRP:CD1 | 2.55 | 0.41 |
| 1:F:54:HIS:HD2 | 1:F:58:ILE:HG12 | 1.86 | 0.41 |
| 2:H:511:TYR:CE2 | 2:H:513:PHE:HB3 | 2.56 | 0.41 |
| 1:A:145:LEU:N | 1:A:145:LEU:HD12 | 2.36 | 0.41 |
| 1:B:116:PHE:HD1 | 1:B:124:LYS:O | 2.03 | 0.41 |
| 2:H:204:PHE:CD1 | 2:H:205:ILE:N | 2.89 | 0.41 |
| 1:F:303:HIS:HD1 | 1:F:325:ASP:CG | 2.23 | 0.41 |
| 2:G:81:PHE:CD1 | 2:G:81:PHE:C | 2.94 | 0.41 |
| 1:B:108:LYS:HE2 | 1:B:133:ILE:HD12 | 2.01 | 0.41 |
| 1:F:226:ARG:HG3 | 1:F:226:ARG:NH1 | 2.33 | 0.41 |
| 1:A:151:THR:CG2 | 1:A:196:ARG:HH22 | 2.33 | 0.41 |
| 1:B:97:ARG:NH1 | 1:B:97:ARG:HG3 | 2.36 | 0.41 |
| 2:C:342:ASN:O | 2:C:343:GLN:C | 2.59 | 0.41 |
| 2:D:218:GLU:HA | 2:D:220:ASP:N | 2.35 | 0.41 |
| 2:D:347:LEU:O | 2:D:348:GLN:C | 2.59 | 0.41 |
| 2:H:209:LEU:HD21 | 2:H:362:LEU:HD11 | 2.02 | 0.41 |
| 2:D:42:PRO:HD2 | 2:D:47:ILE:HA | 2.01 | 0.41 |
| 1:A:245:ILE:HA | 1:A:293:GLN:O | 2.20 | 0.41 |
| 2:G:523:LEU:HD23 | 2:G:538:ILE:HD12 | 2.02 | 0.41 |
| 2:D:253:VAL:HG21 | 2:D:335:PHE:HE1 | 1.85 | 0.41 |
| 2:G:240:PHE:CE2 | 2:G:268:SER:HB2 | 2.56 | 0.41 |
| 2:H:406:LEU:O | 2:H:407:PRO:C | 2.59 | 0.41 |
| 2:H:467:ASN:HA | 2:H:470:ALA:HB3 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:228:TYR:CD2 | 1:A:244:LYS:HG3 | 2.53 | 0.41 |
| 1:F:151:THR:CG2 | 1:F:196:ARG:HH22 | 2.34 | 0.41 |
| 2:G:305:GLU:O | 2:G:308:ASN:HB3 | 2.21 | 0.41 |
| 1:A:113:SER:HB3 | 1:A:170:CYS:HA | 2.03 | 0.41 |
| 1:B:199:ASP:OD2 | 1:B:201:LYS:HD2 | 2.21 | 0.41 |
| 2:D:105:SER:HB2 | 2:D:481:LEU:HD21 | 2.03 | 0.41 |
| 2:G:179:LEU:O | 2:G:182:LEU:N | 2.54 | 0.41 |
| 1:F:313:ASN:HB3 | 1:F:317:THR:H | 1.86 | 0.41 |
| 1:B:6:SER:HB2 | 1:B:8:HIS:HD2 | 1.86 | 0.41 |
| 1:A:74:SER:O | 1:A:81:VAL:HG13 | 2.21 | 0.40 |
| 2:C:253:VAL:HG21 | 2:C:335:PHE:CE1 | 2.56 | 0.40 |
| 2:G:483:PRO:HA | 2:G:521:TRP:HZ2 | 1.86 | 0.40 |
| 2:C:324:ILE:O | 2:C:325:SER:C | 2.60 | 0.40 |
| 2:C:57:PRO:HG2 | 2:C:58:ILE:H | 1.86 | 0.40 |
| 1:B:15:VAL:HB | 2:D:81:PHE:CE2 | 2.56 | 0.40 |
| 1:F:108:LYS:HE2 | 1:F:133:ILE:HD12 | 2.04 | 0.40 |
| 1:F:21:GLY:HA3 | 2:H:73:PRO:HD2 | 2.02 | 0.40 |
| 2:D:543:GLY:O | 2:D:547:LEU:HG | 2.21 | 0.40 |
| 2:C:201:ARG:NH1 | 2:C:201:ARG:HG3 | 2.36 | 0.40 |
| 2:D:367:SER:C | 2:D:369:GLU:N | 2.75 | 0.40 |
| 2:G:248:LEU:HD23 | 2:G:248:LEU:O | 2.21 | 0.40 |
| 2:H:218:GLU:HA | 2:H:220:ASP:N | 2.36 | 0.40 |
| 2:C:218:GLU:HA | 2:C:220:ASP:N | 2.35 | 0.40 |
| 2:G:202:SER:HA | 2:G:297:LYS:O | 2.21 | 0.40 |
| 2:C:91:TYR:N | 2:C:91:TYR:CD1 | 2.89 | 0.40 |
| 2:G:535:ALA:O | 2:G:538:ILE:HB | 2.20 | 0.40 |
| 2:G:86:ASP:CA | 2:G:88:TYR:CE1 | 3.03 | 0.40 |
| 2:C:406:LEU:O | 2:C:407:PRO:C | 2.60 | 0.40 |
| 1:F:82:LYS:HE3 | 1:F:100:LYS:HD3 | 2.02 | 0.40 |
| 1:E:305:GLY:HA3 | 1:E:324:ASP:HB2 | 2.03 | 0.40 |
| 1:E:177:ARG:HD2 | 1:E:178:PHE:CE1 | 2.57 | 0.40 |
| 2:H:205:ILE:O | 2:H:205:ILE:HG22 | 2.21 | 0.40 |
| 2:H:248:LEU:HD23 | 2:H:248:LEU:O | 2.21 | 0.40 |
| 2:H:375:LEU:HB2 | 2:H:398:ILE:HD13 | 2.03 | 0.40 |
| 2:C:86:ASP:CA | 2:C:88:TYR:CE1 | 3.05 | 0.40 |
| 1:A:97:ARG:NH1 | 1:A:97:ARG:HG3 | 2.35 | 0.40 |
| 1:F:97:ARG:NH1 | 1:F:97:ARG:HG3 | 2.36 | 0.40 |
| 2:C:142:ALA:O | 2:C:146:LEU:HG | 2.22 | 0.40 |
| 1:B:2:GLN:HA | 1:B:3:PRO:HD3 | 1.95 | 0.40 |
| 2:C:467:ASN:O | 2:C:471:PHE:CD1 | 2.74 | 0.40 |
| 1:E:25:ALA:O | 1:E:61:ILE:HD12 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:296:PRO:HD3 | 2:D:306:TRP:CD1 | 2.55 | 0.40 |
| 2:D:274:LEU:HD22 | 2:D:281:SER:CB | 2.50 | 0.40 |
| 2:D:200:ASN:O | 2:D:201:ARG:C | 2.60 | 0.40 |
| 1:A:117:ALA:HA | 1:A:173:TRP:CG | 2.56 | 0.40 |
| 1:F:117:ALA:HB2 | 1:F:173:TRP:CE2 | 2.56 | 0.40 |
| 1:F:1:MET:CE | 2:H:94:ARG:HD2 | 2.51 | 0.40 |
| 2:C:85:LYS:O | 2:C:86:ASP:HB2 | 2.21 | 0.40 |
| 1:A:295:GLU:HG2 | 2:D:311:LEU:HD21 | 2.04 | 0.40 |
| 1:F:59:VAL:O | 1:F:59:VAL:HG12 | 2.20 | 0.40 |
| 2:C:558:ASN:CG | 2:C:559:PHE:N | 2.75 | 0.40 |
| 2:D:240:PHE:CE2 | 2:D:268:SER:HB2 | 2.57 | 0.40 |
| 1:F:345:ILE:CD1 | 2:H:93:VAL:HG11 | 2.48 | 0.40 |
| 2:G:467:ASN:O | 2:G:471:PHE:HD1 | 2.05 | 0.40 |
| 1:E:116:PHE:HD1 | 1:E:124:LYS:O | 2.03 | 0.40 |
| 2:H:166:ASP:HB3 | 2:H:169:VAL:HG21 | 2.04 | 0.40 |
| 2:D:67:LEU:HD12 | 2:D:81:PHE:O | 2.22 | 0.40 |
| 2:D:93:VAL:HG12 | 2:D:94:ARG:N | 2.36 | 0.40 |
| 1:B:113:SER:HB3 | 1:B:170:CYS:HA | 2.04 | 0.40 |
| 2:H:367:SER:C | 2:H:369:GLU:N | 2.75 | 0.40 |
| 1:A:1:MET:HE2 | 2:C:94:ARG:HD2 | 2.03 | 0.40 |
| 2:D:508:LEU:C | 2:D:510:HIS:N | 2.75 | 0.40 |
| 1:B:313:ASN:HB3 | 1:B:317:THR:H | 1.86 | 0.40 |
| 1:E:63:TRP:CH2 | 1:E:72:ILE:HD11 | 2.56 | 0.40 |
| 2:D:460:GLY:O | 2:D:462:ALA:N | 2.54 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|---------------|-----------|----------|----------|-------------|
| 1 | A | 294/351 (84%) | 240 (82%) | 48 (16%) | 6 (2%) | 9 54 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1 | B | 294/351 (84%) | 243 (83%) | 45 (15%) | 6 (2%) | 9 | 54 |
| 1 | E | 294/351 (84%) | 242 (82%) | 47 (16%) | 5 (2%) | 11 | 57 |
| 1 | F | 294/351 (84%) | 242 (82%) | 46 (16%) | 6 (2%) | 9 | 54 |
| 2 | C | 486/570 (85%) | 378 (78%) | 82 (17%) | 26 (5%) | 2 | 30 |
| 2 | D | 472/570 (83%) | 371 (79%) | 76 (16%) | 25 (5%) | 2 | 30 |
| 2 | G | 474/570 (83%) | 370 (78%) | 79 (17%) | 25 (5%) | 2 | 30 |
| 2 | H | 487/570 (85%) | 384 (79%) | 78 (16%) | 25 (5%) | 2 | 31 |
| All | All | 3095/3684 (84%) | 2470 (80%) | 501 (16%) | 124 (4%) | 4 | 38 |

All (124) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 302 | ASP |
| 1 | B | 302 | ASP |
| 2 | C | 197 | VAL |
| 2 | C | 200 | ASN |
| 2 | C | 270 | LEU |
| 2 | C | 273 | TYR |
| 2 | D | 43 | VAL |
| 2 | D | 197 | VAL |
| 2 | D | 200 | ASN |
| 2 | D | 270 | LEU |
| 2 | D | 273 | TYR |
| 2 | D | 515 | THR |
| 2 | D | 553 | ILE |
| 1 | E | 302 | ASP |
| 1 | F | 302 | ASP |
| 2 | G | 46 | ALA |
| 2 | G | 197 | VAL |
| 2 | G | 200 | ASN |
| 2 | G | 270 | LEU |
| 2 | G | 273 | TYR |
| 2 | G | 514 | VAL |
| 2 | H | 43 | VAL |
| 2 | H | 197 | VAL |
| 2 | H | 200 | ASN |
| 2 | H | 270 | LEU |
| 2 | H | 273 | TYR |
| 2 | H | 549 | ALA |
| 2 | C | 205 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 235 | ALA |
| 2 | C | 239 | VAL |
| 2 | C | 272 | PRO |
| 2 | C | 479 | LYS |
| 2 | C | 549 | ALA |
| 2 | C | 552 | ILE |
| 2 | C | 556 | ILE |
| 2 | D | 205 | ILE |
| 2 | D | 239 | VAL |
| 2 | D | 272 | PRO |
| 2 | D | 479 | LYS |
| 2 | D | 514 | VAL |
| 2 | G | 205 | ILE |
| 2 | G | 239 | VAL |
| 2 | G | 272 | PRO |
| 2 | G | 493 | ALA |
| 2 | H | 46 | ALA |
| 2 | H | 239 | VAL |
| 2 | H | 272 | PRO |
| 2 | H | 550 | HIS |
| 1 | A | 94 | SER |
| 1 | A | 170 | CYS |
| 1 | B | 170 | CYS |
| 1 | B | 325 | ASP |
| 2 | C | 60 | LYS |
| 2 | C | 101 | SER |
| 2 | C | 543 | GLY |
| 2 | D | 60 | LYS |
| 2 | D | 101 | SER |
| 2 | D | 204 | PHE |
| 2 | D | 461 | MET |
| 2 | D | 493 | ALA |
| 1 | E | 94 | SER |
| 1 | E | 170 | CYS |
| 1 | E | 325 | ASP |
| 1 | F | 94 | SER |
| 1 | F | 170 | CYS |
| 1 | F | 325 | ASP |
| 2 | G | 60 | LYS |
| 2 | G | 101 | SER |
| 2 | G | 204 | PHE |
| 2 | G | 236 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | G | 492 | SER |
| 2 | G | 515 | THR |
| 2 | H | 60 | LYS |
| 2 | H | 101 | SER |
| 2 | H | 204 | PHE |
| 2 | H | 205 | ILE |
| 2 | H | 460 | GLY |
| 2 | H | 479 | LYS |
| 1 | A | 41 | ASP |
| 1 | A | 325 | ASP |
| 1 | B | 41 | ASP |
| 1 | B | 94 | SER |
| 2 | C | 42 | PRO |
| 2 | C | 164 | ASP |
| 2 | C | 172 | PHE |
| 2 | C | 204 | PHE |
| 2 | C | 325 | SER |
| 2 | C | 368 | LEU |
| 2 | D | 164 | ASP |
| 2 | D | 325 | SER |
| 2 | D | 401 | LYS |
| 1 | E | 41 | ASP |
| 1 | F | 41 | ASP |
| 2 | G | 164 | ASP |
| 2 | G | 325 | SER |
| 2 | G | 368 | LEU |
| 2 | H | 164 | ASP |
| 2 | H | 172 | PHE |
| 2 | H | 325 | SER |
| 2 | H | 472 | GLU |
| 2 | C | 119 | GLY |
| 2 | C | 401 | LYS |
| 2 | D | 119 | GLY |
| 2 | D | 172 | PHE |
| 2 | D | 368 | LEU |
| 2 | D | 485 | ALA |
| 2 | G | 119 | GLY |
| 2 | G | 161 | ARG |
| 2 | G | 172 | PHE |
| 2 | H | 368 | LEU |
| 2 | H | 401 | LYS |
| 2 | C | 227 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 227 | VAL |
| 2 | G | 227 | VAL |
| 2 | G | 401 | LYS |
| 2 | H | 119 | GLY |
| 2 | H | 227 | VAL |
| 2 | C | 514 | VAL |
| 2 | C | 553 | ILE |
| 1 | A | 156 | VAL |
| 2 | G | 553 | ILE |
| 2 | H | 527 | VAL |
| 1 | B | 156 | VAL |
| 1 | F | 156 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | A | 262/307 (85%) | 259 (99%) | 3 (1%) | 80 | 92 |
| 1 | B | 262/307 (85%) | 259 (99%) | 3 (1%) | 80 | 92 |
| 1 | E | 262/307 (85%) | 259 (99%) | 3 (1%) | 80 | 92 |
| 1 | F | 262/307 (85%) | 259 (99%) | 3 (1%) | 80 | 92 |
| 2 | C | 438/510 (86%) | 431 (98%) | 7 (2%) | 70 | 90 |
| 2 | D | 428/510 (84%) | 421 (98%) | 7 (2%) | 70 | 90 |
| 2 | G | 429/510 (84%) | 424 (99%) | 5 (1%) | 78 | 91 |
| 2 | H | 439/510 (86%) | 430 (98%) | 9 (2%) | 61 | 86 |
| All | All | 2782/3268 (85%) | 2742 (99%) | 40 (1%) | 74 | 90 |

All (40) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 5 | ASP |
| 1 | A | 171 | LEU |
| 1 | A | 226 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 5 | ASP |
| 1 | B | 171 | LEU |
| 1 | B | 226 | ARG |
| 2 | C | 200 | ASN |
| 2 | C | 269 | ASP |
| 2 | C | 308 | ASN |
| 2 | C | 465 | MET |
| 2 | C | 488 | LEU |
| 2 | C | 497 | ARG |
| 2 | C | 558 | ASN |
| 2 | D | 200 | ASN |
| 2 | D | 269 | ASP |
| 2 | D | 308 | ASN |
| 2 | D | 497 | ARG |
| 2 | D | 518 | ASP |
| 2 | D | 530 | ARG |
| 2 | D | 533 | GLU |
| 1 | E | 5 | ASP |
| 1 | E | 171 | LEU |
| 1 | E | 226 | ARG |
| 1 | F | 5 | ASP |
| 1 | F | 171 | LEU |
| 1 | F | 226 | ARG |
| 2 | G | 200 | ASN |
| 2 | G | 269 | ASP |
| 2 | G | 308 | ASN |
| 2 | G | 457 | TYR |
| 2 | G | 533 | GLU |
| 2 | H | 200 | ASN |
| 2 | H | 231 | LYS |
| 2 | H | 269 | ASP |
| 2 | H | 308 | ASN |
| 2 | H | 459 | ASN |
| 2 | H | 497 | ARG |
| 2 | H | 518 | ASP |
| 2 | H | 533 | GLU |
| 2 | H | 558 | ASN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 308 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 545 | GLN |
| 2 | D | 308 | ASN |
| 2 | G | 551 | ASN |
| 2 | H | 308 | 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 carbohydrates 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 | 300/351 (85%) | 0.34 | 6 (2%) 68 53 | 97, 126, 151, 158 | 0 |
| 1 | B | 300/351 (85%) | 0.33 | 8 (2%) 58 42 | 96, 125, 152, 160 | 0 |
| 1 | E | 300/351 (85%) | 0.28 | 11 (3%) 45 31 | 97, 126, 152, 160 | 0 |
| 1 | F | 300/351 (85%) | 0.35 | 10 (3%) 50 35 | 98, 126, 151, 158 | 0 |
| 2 | C | 492/570 (86%) | 0.11 | 13 (2%) 59 43 | 90, 124, 170, 179 | 0 |
| 2 | D | 480/570 (84%) | 0.05 | 6 (1%) 79 65 | 92, 122, 167, 180 | 0 |
| 2 | G | 482/570 (84%) | 0.08 | 6 (1%) 81 67 | 92, 123, 167, 179 | 0 |
| 2 | H | 493/570 (86%) | 0.18 | 6 (1%) 81 67 | 91, 125, 170, 183 | 0 |
| All | All | 3147/3684 (85%) | 0.19 | 66 (2%) 67 51 | 90, 124, 162, 183 | 0 |

All (66) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | D | 126 | VAL | 6.4 |
| 2 | G | 61 | ASN | 5.0 |
| 2 | C | 124 | PHE | 4.8 |
| 2 | H | 121 | ASP | 4.0 |
| 1 | F | 195 | GLN | 3.9 |
| 1 | B | 167 | SER | 3.9 |
| 1 | B | 168 | ASP | 3.8 |
| 2 | G | 136 | PHE | 3.8 |
| 2 | C | 121 | ASP | 3.2 |
| 2 | C | 122 | ARG | 3.2 |
| 1 | E | 306 | GLU | 3.0 |
| 2 | H | 124 | PHE | 2.9 |
| 1 | B | 307 | VAL | 2.9 |
| 2 | H | 430 | ILE | 2.9 |
| 2 | C | 136 | PHE | 2.9 |
| 1 | B | 160 | PRO | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | F | 75 | ALA | 2.8 |
| 2 | C | 141 | ASN | 2.8 |
| 2 | C | 67 | LEU | 2.7 |
| 2 | H | 61 | ASN | 2.7 |
| 1 | E | 160 | PRO | 2.7 |
| 2 | G | 227 | VAL | 2.7 |
| 1 | F | 112 | TYR | 2.7 |
| 1 | E | 169 | PHE | 2.6 |
| 1 | A | 195 | GLN | 2.6 |
| 1 | F | 45 | TRP | 2.6 |
| 2 | C | 139 | GLU | 2.5 |
| 2 | C | 454 | LEU | 2.5 |
| 1 | A | 145 | LEU | 2.4 |
| 2 | C | 366 | PRO | 2.4 |
| 1 | F | 199 | ASP | 2.4 |
| 1 | E | 188 | LEU | 2.3 |
| 1 | F | 167 | SER | 2.3 |
| 1 | F | 290 | SER | 2.3 |
| 2 | D | 71 | LEU | 2.3 |
| 1 | F | 208 | LEU | 2.3 |
| 1 | A | 71 | ILE | 2.3 |
| 1 | E | 168 | ASP | 2.3 |
| 2 | C | 193 | ASP | 2.3 |
| 1 | E | 307 | VAL | 2.3 |
| 1 | B | 170 | CYS | 2.2 |
| 2 | D | 136 | PHE | 2.2 |
| 1 | B | 191 | ALA | 2.2 |
| 2 | C | 140 | HIS | 2.2 |
| 2 | D | 219 | PRO | 2.2 |
| 1 | F | 171 | LEU | 2.2 |
| 2 | C | 125 | ASN | 2.1 |
| 1 | E | 75 | ALA | 2.1 |
| 1 | F | 343 | SER | 2.1 |
| 2 | C | 65 | MET | 2.1 |
| 2 | G | 126 | VAL | 2.1 |
| 1 | E | 214 | LEU | 2.1 |
| 2 | H | 138 | LYS | 2.1 |
| 1 | E | 124 | LYS | 2.1 |
| 2 | G | 168 | ARG | 2.1 |
| 1 | A | 208 | LEU | 2.1 |
| 1 | B | 53 | ALA | 2.1 |
| 2 | H | 62 | GLY | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | D | 61 | ASN | 2.1 |
| 2 | D | 193 | ASP | 2.1 |
| 1 | E | 193 | ILE | 2.0 |
| 1 | A | 167 | SER | 2.0 |
| 2 | G | 62 | GLY | 2.0 |
| 1 | B | 232 | ALA | 2.0 |
| 1 | E | 170 | CYS | 2.0 |
| 1 | A | 240 | ILE | 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 carbohydrates 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.