



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 10:21 am BST

PDB ID : 3P03
Title : Crystal structure of BetP-G153D with choline bound
Authors : Perez, C.; Ressler, S.; Ziegler, Z.
Deposited on : 2010-09-27
Resolution : 3.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

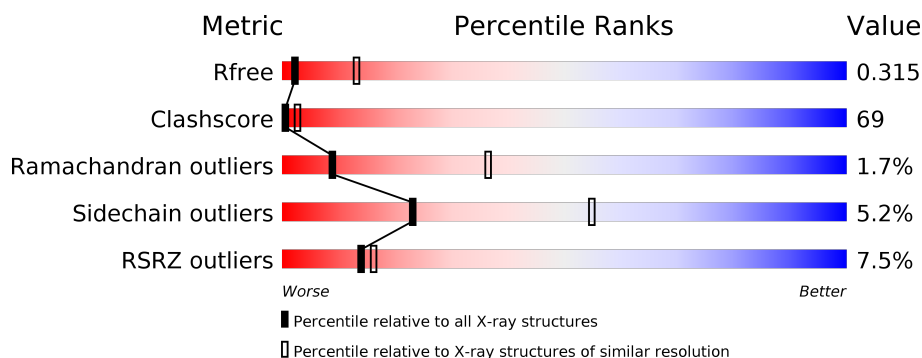
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1558 (3.42-3.30) |
| Clashscore | 141614 | 1627 (3.42-3.30) |
| Ramachandran outliers | 138981 | 1599 (3.42-3.30) |
| Sidechain outliers | 138945 | 1598 (3.42-3.30) |
| RSRZ outliers | 127900 | 1507 (3.42-3.30) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 566 | |
| 1 | B | 566 | |
| 1 | C | 566 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2 | CHT | C | 2486 | - | - | X | X |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11349 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.

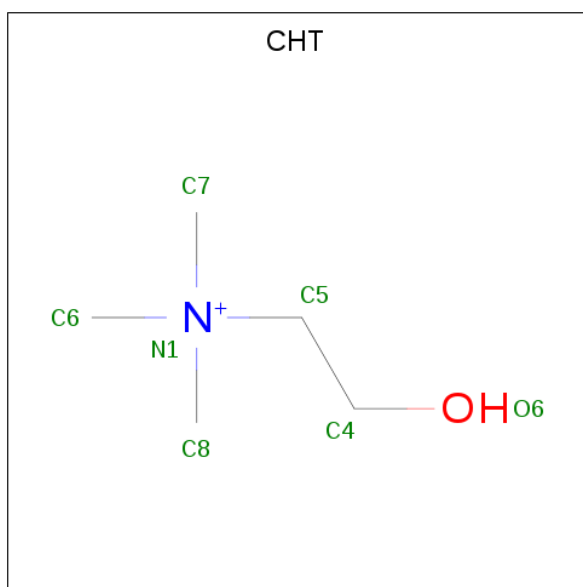
- Molecule 1 is a protein called Glycine betaine transporter BetP.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3868 | 2542 | 641 | 669 | 16 | | | |
| 1 | B | 476 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3612 | 2391 | 577 | 628 | 16 | | | |
| 1 | C | 508 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3862 | 2545 | 627 | 674 | 16 | | | |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 44 | ALA | GLU | ENGINEERED MUTATION | UNP P54582 |
| A | 45 | ALA | GLU | ENGINEERED MUTATION | UNP P54582 |
| A | 46 | ALA | GLU | ENGINEERED MUTATION | UNP P54582 |
| A | 153 | ASP | GLY | ENGINEERED MUTATION | UNP P54582 |
| B | 44 | ALA | GLU | ENGINEERED MUTATION | UNP P54582 |
| B | 45 | ALA | GLU | ENGINEERED MUTATION | UNP P54582 |
| B | 46 | ALA | GLU | ENGINEERED MUTATION | UNP P54582 |
| B | 153 | ASP | GLY | ENGINEERED MUTATION | UNP P54582 |
| C | 44 | ALA | GLU | ENGINEERED MUTATION | UNP P54582 |
| C | 45 | ALA | GLU | ENGINEERED MUTATION | UNP P54582 |
| C | 46 | ALA | GLU | ENGINEERED MUTATION | UNP P54582 |
| C | 153 | ASP | GLY | ENGINEERED MUTATION | UNP P54582 |

- Molecule 2 is CHOLINE ION (three-letter code: CHT) (formula: C₅H₁₄NO).

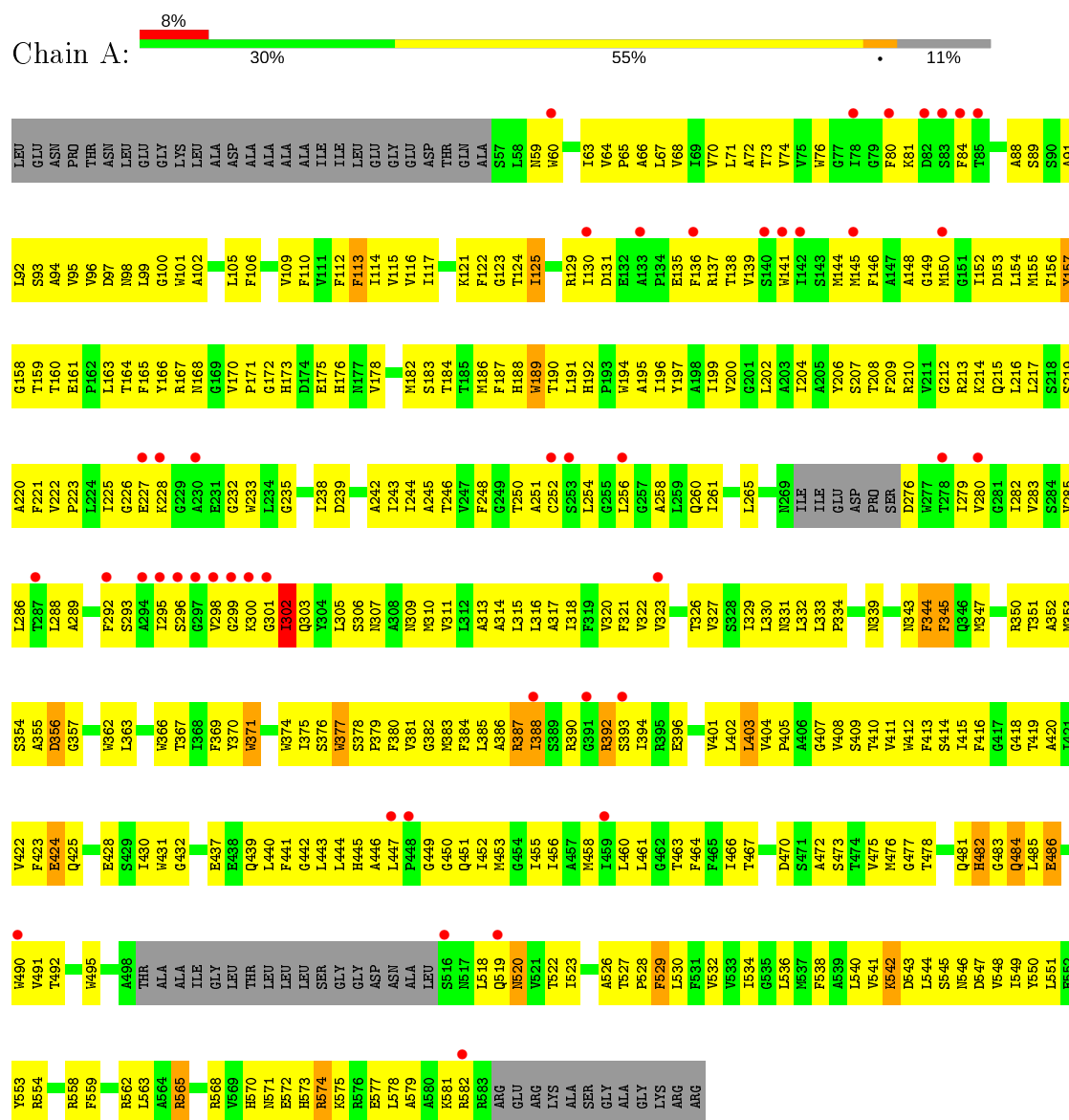


| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| | | | Total | C | N | O | | |
| 2 | C | 1 | 7 | 5 | 1 | 1 | 0 | 0 |

3 Residue-property plots

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

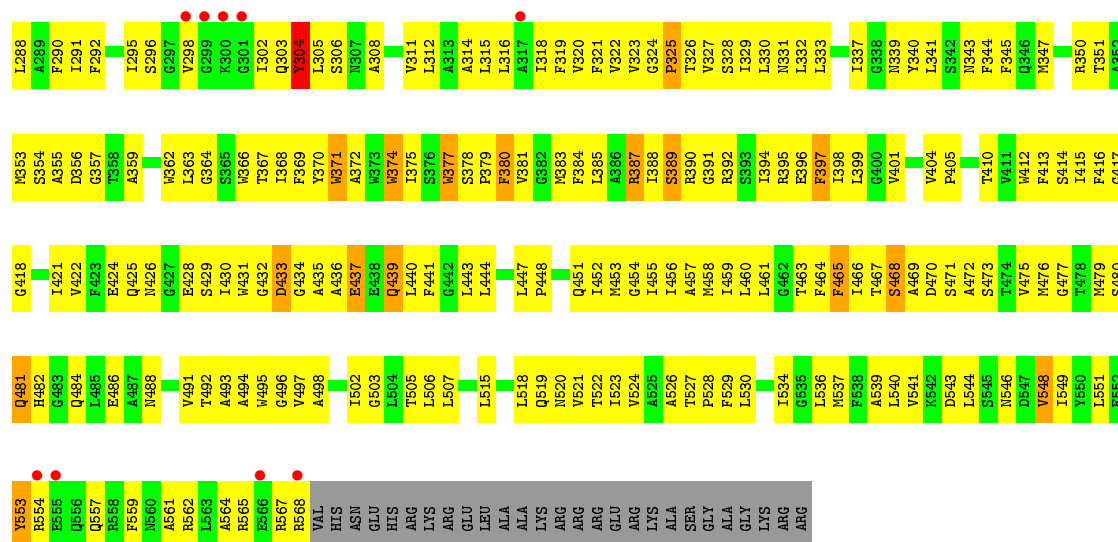
• Molecule 1: Glycine betaine transporter BetP



• Molecule 1: Glycine betaine transporter BetP







4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 117.56Å 129.31Å 183.14Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 46.20 – 3.35 48.18 – 3.30 | Depositor EDS |
| % Data completeness (in resolution range) | 91.2 (46.20-3.35) 87.6 (48.18-3.30) | Depositor EDS |
| R_{merge} | 0.13 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 15.91 (at 3.33Å) | Xtriage |
| Refinement program | PHENIX 1.6.2_432 | Depositor |
| R, R_{free} | 0.245 , 0.300 0.276 , 0.315 | Depositor DCC |
| R_{free} test set | 3712 reflections (9.95%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 70.2 | Xtriage |
| Anisotropy | 0.012 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 105.3 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.83 | EDS |
| Total number of atoms | 11349 | wwPDB-VP |
| Average B, all atoms (Å ²) | 107.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CHT

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 | 0.33 | 0/3967 | 0.56 | 1/5397 (0.0%) |
| 1 | B | 0.37 | 0/3706 | 0.59 | 0/5051 |
| 1 | C | 0.44 | 0/3960 | 0.64 | 0/5396 |
| All | All | 0.38 | 0/11633 | 0.59 | 1/15844 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|-----|------|--------|-------|------------------------|---------------------|
| 1 | A | 367 | THR | C-N-CA | -5.06 | 109.06 | 121.70 |

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 | 3868 | 0 | 3897 | 495 | 0 |
| 1 | B | 3612 | 0 | 3647 | 542 | 0 |
| 1 | C | 3862 | 0 | 3899 | 579 | 0 |
| 2 | C | 7 | 0 | 14 | 6 | 0 |
| All | All | 11349 | 0 | 11457 | 1576 | 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 69.

All (1576) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:170:VAL:CG1 | 1:C:171:PRO:HD2 | 1.50 | 1.41 |
| 1:C:226:GLY:HA2 | 1:C:227:GLU:CB | 1.47 | 1.40 |
| 1:C:247:VAL:HG12 | 1:C:502:ILE:CD1 | 1.54 | 1.35 |
| 1:B:69:ILE:O | 1:B:73:THR:HG23 | 1.33 | 1.29 |
| 1:B:208:THR:HG22 | 1:B:213:ARG:O | 1.32 | 1.27 |
| 1:C:173:HIS:HD2 | 1:C:180:VAL:CG1 | 1.47 | 1.25 |
| 1:C:363:LEU:CD2 | 1:C:367:THR:HG21 | 1.66 | 1.24 |
| 1:A:369:PHE:CE1 | 1:A:519:GLN:HB2 | 1.72 | 1.24 |
| 1:C:64:VAL:CG1 | 1:C:65:PRO:HD3 | 1.67 | 1.23 |
| 1:C:173:HIS:CD2 | 1:C:180:VAL:HG11 | 1.72 | 1.23 |
| 1:C:247:VAL:CG1 | 1:C:502:ILE:HD11 | 1.68 | 1.22 |
| 1:C:148:ALA:O | 2:C:2486:CHT:H62 | 1.26 | 1.22 |
| 1:A:153:ASP:HA | 1:A:156:PHE:CE2 | 1.79 | 1.17 |
| 1:C:64:VAL:HG13 | 1:C:65:PRO:HD3 | 1.22 | 1.17 |
| 1:B:309:ASN:ND2 | 1:B:464:PHE:HD2 | 1.41 | 1.16 |
| 1:A:418:GLY:O | 1:A:422:VAL:HG23 | 1.41 | 1.15 |
| 1:C:173:HIS:CD2 | 1:C:180:VAL:CG1 | 2.27 | 1.15 |
| 1:C:170:VAL:HG12 | 1:C:171:PRO:CD | 1.76 | 1.15 |
| 1:C:247:VAL:CG1 | 1:C:502:ILE:CD1 | 2.24 | 1.15 |
| 1:A:559:PHE:CE2 | 1:A:563:LEU:HD12 | 1.82 | 1.15 |
| 1:C:304:TYR:HD1 | 1:C:305:LEU:N | 1.45 | 1.14 |
| 1:C:134:PRO:HA | 1:C:391:GLY:HA3 | 1.31 | 1.12 |
| 1:A:343:ASN:O | 1:A:347:MET:HG3 | 1.46 | 1.12 |
| 1:C:261:ILE:HD11 | 1:C:461:LEU:HB2 | 1.25 | 1.12 |
| 1:B:398:ILE:O | 1:B:402:LEU:HD13 | 1.49 | 1.12 |
| 1:B:201:GLY:HA3 | 1:B:385:LEU:HD11 | 1.26 | 1.11 |
| 1:A:369:PHE:CZ | 1:A:519:GLN:HB2 | 1.85 | 1.11 |
| 1:C:105:LEU:O | 1:C:109:VAL:HG23 | 1.51 | 1.11 |
| 1:B:343:ASN:O | 1:B:347:MET:HG2 | 1.51 | 1.10 |
| 1:C:226:GLY:CA | 1:C:227:GLU:HB3 | 1.82 | 1.10 |
| 1:C:363:LEU:HD22 | 1:C:367:THR:HG21 | 1.09 | 1.09 |
| 1:C:144:MET:HG2 | 1:C:388:ILE:HD11 | 1.19 | 1.09 |
| 1:A:60:TRP:HA | 1:A:63:ILE:HG22 | 1.27 | 1.09 |
| 1:B:92:LEU:HD11 | 1:B:523:ILE:HB | 1.33 | 1.08 |
| 1:B:190:THR:O | 1:B:194:TRP:HD1 | 1.34 | 1.08 |
| 1:B:196:ILE:HD11 | 1:B:374:TRP:HB3 | 1.34 | 1.07 |
| 1:C:237:LEU:O | 1:C:240:ILE:HG22 | 1.55 | 1.07 |
| 1:B:312:LEU:HB3 | 1:B:460:LEU:HD21 | 1.12 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:570:HIS:O | 1:A:574:ARG:HD3 | 1.55 | 1.06 |
| 1:C:173:HIS:HD2 | 1:C:180:VAL:HG11 | 0.99 | 1.06 |
| 1:A:351:THR:CG2 | 1:C:331:ASN:HB3 | 1.85 | 1.06 |
| 1:B:309:ASN:OD1 | 1:B:463:THR:HG21 | 1.56 | 1.06 |
| 1:C:226:GLY:CA | 1:C:227:GLU:CB | 2.31 | 1.06 |
| 1:A:89:SER:HA | 1:A:520:ASN:HD21 | 1.20 | 1.05 |
| 1:C:226:GLY:HA2 | 1:C:227:GLU:HB3 | 1.10 | 1.04 |
| 1:B:208:THR:O | 1:B:212:GLY:HA2 | 1.57 | 1.04 |
| 1:B:200:VAL:HG21 | 1:B:378:SER:HB3 | 1.04 | 1.04 |
| 1:C:304:TYR:CE1 | 1:C:305:LEU:HG | 1.93 | 1.03 |
| 1:C:224:LEU:HD11 | 1:C:539:ALA:N | 1.71 | 1.03 |
| 1:B:312:LEU:HB3 | 1:B:460:LEU:CD2 | 1.87 | 1.03 |
| 1:A:123:GLY:HA2 | 1:A:394:ILE:HB | 1.37 | 1.03 |
| 1:B:114:ILE:O | 1:B:117:ILE:HG22 | 1.58 | 1.03 |
| 1:C:144:MET:HG2 | 1:C:388:ILE:CD1 | 1.88 | 1.03 |
| 1:C:375:ILE:HD13 | 1:C:530:LEU:HA | 1.39 | 1.02 |
| 1:A:478:THR:HA | 1:A:481:GLN:NE2 | 1.72 | 1.02 |
| 1:A:329:ILE:HD11 | 1:A:419:THR:CG2 | 1.89 | 1.02 |
| 1:B:369:PHE:CD1 | 1:B:523:ILE:HD11 | 1.95 | 1.02 |
| 1:C:363:LEU:HA | 1:C:367:THR:HG22 | 1.40 | 1.01 |
| 1:A:412:TRP:CE2 | 1:A:416:PHE:CE2 | 2.48 | 1.01 |
| 1:C:188:HIS:CG | 1:C:370:TYR:CD2 | 2.49 | 1.01 |
| 1:C:224:LEU:HD11 | 1:C:539:ALA:CA | 1.89 | 1.01 |
| 1:C:226:GLY:HA2 | 1:C:227:GLU:HB2 | 1.32 | 1.01 |
| 1:C:126:ARG:HD3 | 1:C:132:GLU:O | 1.61 | 1.01 |
| 1:C:163:LEU:HG | 1:C:431:TRP:HZ3 | 1.22 | 1.00 |
| 1:C:343:ASN:O | 1:C:347:MET:HG2 | 1.60 | 1.00 |
| 1:A:64:VAL:HG23 | 1:A:65:PRO:HD3 | 1.44 | 1.00 |
| 1:C:295:ILE:HD11 | 1:C:493:ALA:HB2 | 1.38 | 1.00 |
| 1:C:76:TRP:HE1 | 1:C:85:THR:CB | 1.73 | 1.00 |
| 1:A:412:TRP:CZ2 | 1:A:416:PHE:CE2 | 2.50 | 0.99 |
| 1:C:108:THR:HA | 1:C:192:HIS:CE1 | 1.97 | 0.99 |
| 1:C:91:ALA:O | 1:C:94:ALA:HB3 | 1.61 | 0.99 |
| 1:A:310:MET:O | 1:A:314:ALA:HB3 | 1.63 | 0.99 |
| 1:A:481:GLN:O | 1:A:482:HIS:HB2 | 1.62 | 0.98 |
| 1:B:200:VAL:HG11 | 1:B:378:SER:O | 1.64 | 0.98 |
| 1:C:121:LYS:H | 1:C:121:LYS:HD3 | 1.28 | 0.98 |
| 1:B:366:TRP:O | 1:B:370:TYR:HB2 | 1.63 | 0.98 |
| 1:A:559:PHE:HE2 | 1:A:563:LEU:HD12 | 1.12 | 0.98 |
| 1:C:76:TRP:HE1 | 1:C:85:THR:CA | 1.76 | 0.97 |
| 1:A:351:THR:HG21 | 1:C:331:ASN:HB3 | 1.43 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:81:LYS:HB2 | 1:A:84:PHE:HB2 | 1.46 | 0.97 |
| 1:B:473:SER:HB2 | 1:B:492:THR:O | 1.63 | 0.97 |
| 1:C:188:HIS:CD2 | 1:C:370:TYR:CD2 | 2.53 | 0.97 |
| 1:C:61:SER:O | 1:C:65:PRO:HG2 | 1.64 | 0.97 |
| 1:B:110:PHE:CD1 | 1:B:196:ILE:HG22 | 2.01 | 0.96 |
| 1:A:215:GLN:HB3 | 1:A:483:GLY:O | 1.65 | 0.96 |
| 1:A:60:TRP:HA | 1:A:63:ILE:CG2 | 1.95 | 0.96 |
| 1:C:81:LYS:HB3 | 1:C:84:PHE:HD2 | 1.29 | 0.96 |
| 1:C:188:HIS:CD2 | 1:C:370:TYR:HD2 | 1.84 | 0.95 |
| 1:C:92:LEU:HD13 | 1:C:520:ASN:HA | 1.48 | 0.95 |
| 1:C:304:TYR:CD1 | 1:C:305:LEU:N | 2.35 | 0.95 |
| 1:A:113:PHE:CE1 | 1:A:117:ILE:HD11 | 2.02 | 0.95 |
| 1:A:153:ASP:HA | 1:A:156:PHE:HE2 | 1.16 | 0.94 |
| 1:B:320:VAL:HG23 | 1:B:415:ILE:CG2 | 1.98 | 0.94 |
| 1:B:114:ILE:HA | 1:B:117:ILE:HG22 | 1.48 | 0.94 |
| 1:B:129:ARG:H | 1:B:390:ARG:HH12 | 1.03 | 0.94 |
| 1:C:329:ILE:HD13 | 1:C:415:ILE:HG23 | 1.47 | 0.94 |
| 1:C:210:ARG:HH22 | 1:C:549:ILE:HD12 | 1.30 | 0.94 |
| 1:B:327:VAL:HG23 | 1:B:328:SER:H | 1.30 | 0.94 |
| 1:B:488:ASN:OD1 | 1:B:490:TRP:HZ3 | 1.47 | 0.94 |
| 1:C:170:VAL:CG1 | 1:C:171:PRO:CD | 2.41 | 0.93 |
| 1:A:344:PHE:HD2 | 1:A:344:PHE:C | 1.70 | 0.93 |
| 1:A:445:HIS:HA | 1:A:450:GLY:HA3 | 1.50 | 0.93 |
| 1:B:327:VAL:HG23 | 1:B:328:SER:N | 1.82 | 0.93 |
| 1:B:411:VAL:O | 1:B:415:ILE:HD12 | 1.68 | 0.93 |
| 1:A:309:ASN:CG | 1:A:464:PHE:HE1 | 1.70 | 0.93 |
| 1:C:260:GLN:CD | 1:C:461:LEU:HD21 | 1.89 | 0.92 |
| 1:A:305:LEU:HD22 | 1:A:467:THR:HG22 | 1.52 | 0.92 |
| 1:B:200:VAL:CG2 | 1:B:378:SER:HB3 | 1.99 | 0.92 |
| 1:B:186:MET:O | 1:B:190:THR:HG23 | 1.69 | 0.92 |
| 1:B:411:VAL:HG13 | 1:B:415:ILE:CD1 | 2.00 | 0.92 |
| 1:C:144:MET:CG | 1:C:388:ILE:CD1 | 2.46 | 0.92 |
| 1:B:92:LEU:CD1 | 1:B:523:ILE:HB | 1.99 | 0.92 |
| 1:C:170:VAL:HG12 | 1:C:171:PRO:HD2 | 0.92 | 0.92 |
| 1:C:81:LYS:HB3 | 1:C:84:PHE:CD2 | 2.05 | 0.92 |
| 1:C:76:TRP:HE1 | 1:C:85:THR:HA | 1.32 | 0.91 |
| 1:B:125:ILE:HG21 | 1:B:210:ARG:NH2 | 1.85 | 0.91 |
| 1:C:363:LEU:HD22 | 1:C:367:THR:CG2 | 1.97 | 0.91 |
| 1:B:186:MET:HG2 | 1:B:190:THR:HG21 | 1.52 | 0.91 |
| 1:C:64:VAL:HG13 | 1:C:65:PRO:CD | 2.00 | 0.91 |
| 1:C:261:ILE:HD11 | 1:C:461:LEU:CB | 2.01 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:144:MET:CG | 1:C:388:ILE:HD11 | 2.00 | 0.90 |
| 1:A:344:PHE:C | 1:A:344:PHE:CD2 | 2.40 | 0.90 |
| 1:C:381:VAL:HG12 | 1:C:385:LEU:HD12 | 1.54 | 0.90 |
| 1:A:527:THR:N | 1:A:528:PRO:HD2 | 1.87 | 0.89 |
| 1:C:209:PHE:CZ | 1:C:390:ARG:HB2 | 2.07 | 0.89 |
| 1:B:370:TYR:O | 1:B:374:TRP:CD1 | 2.25 | 0.89 |
| 1:C:76:TRP:NE1 | 1:C:85:THR:HA | 1.86 | 0.89 |
| 1:B:114:ILE:CA | 1:B:117:ILE:HG22 | 2.03 | 0.89 |
| 1:B:74:VAL:O | 1:B:78:ILE:HG12 | 1.73 | 0.89 |
| 1:B:316:LEU:HD22 | 1:B:460:LEU:CD1 | 2.01 | 0.89 |
| 1:C:103:PHE:CE2 | 1:C:530:LEU:CD2 | 2.56 | 0.89 |
| 1:B:161:GLU:HG2 | 1:B:185:THR:OG1 | 1.74 | 0.88 |
| 1:B:524:VAL:HA | 1:B:527:THR:OG1 | 1.72 | 0.88 |
| 1:C:170:VAL:HG13 | 1:C:171:PRO:HD2 | 1.55 | 0.88 |
| 1:B:460:LEU:O | 1:B:463:THR:HG22 | 1.72 | 0.88 |
| 1:C:188:HIS:CG | 1:C:370:TYR:CE2 | 2.62 | 0.88 |
| 1:C:103:PHE:CE2 | 1:C:530:LEU:HD22 | 2.08 | 0.88 |
| 1:B:196:ILE:CD1 | 1:B:374:TRP:HB3 | 2.04 | 0.88 |
| 1:A:310:MET:O | 1:A:314:ALA:CB | 2.21 | 0.87 |
| 1:C:247:VAL:CG1 | 1:C:502:ILE:HD13 | 2.04 | 0.87 |
| 1:B:69:ILE:O | 1:B:73:THR:CG2 | 2.21 | 0.87 |
| 1:C:114:ILE:HD12 | 1:C:117:ILE:HD11 | 1.55 | 0.87 |
| 1:C:250:THR:HG22 | 1:C:377:TRP:HE1 | 1.37 | 0.87 |
| 1:B:158:GLY:HA2 | 1:B:413:PHE:CE1 | 2.09 | 0.87 |
| 1:C:363:LEU:CD2 | 1:C:367:THR:CG2 | 2.53 | 0.86 |
| 1:A:292:PHE:O | 1:A:296:SER:HB3 | 1.76 | 0.86 |
| 1:A:156:PHE:CE1 | 1:A:157:TYR:CD2 | 2.64 | 0.86 |
| 1:C:247:VAL:HG12 | 1:C:502:ILE:HD11 | 0.88 | 0.86 |
| 1:A:209:PHE:CD2 | 1:A:390:ARG:HG2 | 2.10 | 0.86 |
| 1:B:78:ILE:HG22 | 1:B:79:GLY:N | 1.90 | 0.85 |
| 1:A:574:ARG:N | 1:A:574:ARG:CD | 2.39 | 0.85 |
| 1:B:101:TRP:HA | 1:B:104:ILE:HD11 | 1.57 | 0.85 |
| 1:B:92:LEU:CD1 | 1:B:524:VAL:HG13 | 2.06 | 0.85 |
| 1:C:228:LYS:O | 1:C:228:LYS:HG2 | 1.77 | 0.85 |
| 1:B:317:ALA:O | 1:B:320:VAL:HG22 | 1.77 | 0.85 |
| 1:B:320:VAL:CG2 | 1:B:415:ILE:CG2 | 2.53 | 0.85 |
| 1:C:64:VAL:HG12 | 1:C:65:PRO:HD3 | 1.55 | 0.85 |
| 1:B:78:ILE:HG22 | 1:B:79:GLY:H | 1.41 | 0.85 |
| 1:C:148:ALA:O | 2:C:2486:CHT:C6 | 2.21 | 0.85 |
| 1:A:527:THR:HG22 | 1:A:528:PRO:HD3 | 1.55 | 0.84 |
| 1:B:95:VAL:HG21 | 1:B:527:THR:CG2 | 2.08 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:260:GLN:HA | 1:A:437:GLU:HG2 | 1.57 | 0.84 |
| 1:A:222:VAL:HB | 1:A:227:GLU:HA | 1.59 | 0.84 |
| 1:A:215:GLN:CB | 1:A:483:GLY:O | 2.24 | 0.84 |
| 1:C:311:VAL:HG23 | 1:C:312:LEU:HD12 | 1.60 | 0.84 |
| 1:B:146:PHE:HB3 | 1:B:310:MET:SD | 2.18 | 0.84 |
| 1:B:372:ALA:CB | 1:B:523:ILE:HG23 | 2.07 | 0.84 |
| 1:C:167:ARG:HG3 | 1:C:168:ASN:OD1 | 1.78 | 0.84 |
| 1:B:319:PHE:O | 1:B:323:VAL:HG22 | 1.77 | 0.84 |
| 1:B:205:ALA:HB2 | 1:B:386:ALA:HB1 | 1.60 | 0.84 |
| 1:B:183:SER:OG | 1:B:339:ASN:HB3 | 1.78 | 0.83 |
| 1:B:411:VAL:HG13 | 1:B:415:ILE:HD11 | 1.57 | 0.83 |
| 1:B:190:THR:O | 1:B:194:TRP:CD1 | 2.26 | 0.83 |
| 1:C:173:HIS:HD2 | 1:C:180:VAL:HG13 | 1.43 | 0.83 |
| 1:C:397:PHE:O | 1:C:401:VAL:HG23 | 1.77 | 0.83 |
| 1:A:369:PHE:HE1 | 1:A:519:GLN:HB2 | 1.33 | 0.83 |
| 1:C:224:LEU:HD12 | 1:C:539:ALA:HB2 | 1.59 | 0.83 |
| 1:A:123:GLY:HA2 | 1:A:394:ILE:CB | 2.08 | 0.83 |
| 1:C:267:ALA:HB1 | 1:C:451:GLN:OE1 | 1.77 | 0.83 |
| 1:B:211:VAL:HG11 | 1:B:213:ARG:HE | 1.44 | 0.83 |
| 1:C:337:ILE:HD11 | 1:C:410:THR:HG21 | 1.60 | 0.83 |
| 1:B:488:ASN:OD1 | 1:B:490:TRP:CZ3 | 2.30 | 0.83 |
| 1:C:329:ILE:HG21 | 1:C:415:ILE:HG12 | 1.61 | 0.83 |
| 1:C:103:PHE:CD2 | 1:C:530:LEU:HD22 | 2.13 | 0.83 |
| 1:C:126:ARG:CD | 1:C:132:GLU:O | 2.26 | 0.83 |
| 1:C:163:LEU:HG | 1:C:431:TRP:CZ3 | 2.11 | 0.83 |
| 1:A:331:ASN:O | 1:A:334:PRO:HD2 | 1.78 | 0.82 |
| 1:C:120:SER:HG | 1:C:122:PHE:HD2 | 1.26 | 0.82 |
| 1:A:559:PHE:HE2 | 1:A:563:LEU:CD1 | 1.91 | 0.82 |
| 1:C:121:LYS:CD | 1:C:121:LYS:H | 1.88 | 0.82 |
| 1:C:173:HIS:CD2 | 1:C:180:VAL:CG2 | 2.62 | 0.82 |
| 1:C:134:PRO:HG3 | 1:C:391:GLY:O | 1.79 | 0.82 |
| 1:A:89:SER:HA | 1:A:520:ASN:ND2 | 1.93 | 0.82 |
| 1:C:192:HIS:N | 1:C:193:PRO:HD2 | 1.95 | 0.82 |
| 1:B:153:ASP:OD1 | 1:B:154:LEU:N | 2.12 | 0.81 |
| 1:A:352:ALA:O | 1:A:357:GLY:HA2 | 1.79 | 0.81 |
| 1:B:309:ASN:OD1 | 1:B:463:THR:CG2 | 2.27 | 0.81 |
| 1:C:204:ILE:HD13 | 1:C:383:MET:HG2 | 1.59 | 0.81 |
| 1:C:298:VAL:HG23 | 1:C:302:ILE:HD13 | 1.60 | 0.81 |
| 1:C:252:CYS:SG | 1:C:522:THR:HG21 | 2.20 | 0.81 |
| 1:C:319:PHE:CE2 | 1:C:453:MET:HG3 | 2.15 | 0.81 |
| 1:C:74:VAL:HA | 1:C:505:THR:HG21 | 1.62 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:295:ILE:CD1 | 1:C:493:ALA:HB2 | 2.10 | 0.81 |
| 1:A:302:ILE:CG1 | 1:A:303:GLN:N | 2.42 | 0.81 |
| 1:A:490:TRP:HD1 | 1:A:491:VAL:HG13 | 1.44 | 0.81 |
| 1:A:101:TRP:CE2 | 1:C:330:LEU:HD13 | 2.16 | 0.81 |
| 1:A:299:GLY:O | 1:A:300:LYS:HB2 | 1.81 | 0.81 |
| 1:B:464:PHE:HA | 1:B:467:THR:HG23 | 1.62 | 0.81 |
| 1:B:305:LEU:HD23 | 1:B:467:THR:HG22 | 1.61 | 0.81 |
| 1:C:116:VAL:O | 1:C:120:SER:HB3 | 1.80 | 0.80 |
| 1:B:114:ILE:C | 1:B:117:ILE:HG22 | 2.01 | 0.80 |
| 1:C:103:PHE:HZ | 1:C:527:THR:HA | 1.46 | 0.80 |
| 1:A:343:ASN:O | 1:A:347:MET:CG | 2.29 | 0.80 |
| 1:A:92:LEU:O | 1:A:95:VAL:HG22 | 1.81 | 0.80 |
| 1:B:373:TRP:CD1 | 1:B:373:TRP:C | 2.55 | 0.80 |
| 1:A:113:PHE:CE1 | 1:A:117:ILE:CD1 | 2.66 | 0.80 |
| 1:B:366:TRP:O | 1:B:370:TYR:CB | 2.30 | 0.80 |
| 1:C:228:LYS:O | 1:C:228:LYS:CG | 2.30 | 0.80 |
| 1:A:137:ARG:HD2 | 1:A:139:VAL:HG22 | 1.64 | 0.79 |
| 1:B:103:PHE:HD1 | 1:B:371:TRP:CB | 1.95 | 0.79 |
| 1:C:190:THR:O | 1:C:193:PRO:HG2 | 1.82 | 0.79 |
| 1:C:524:VAL:O | 1:C:528:PRO:HD3 | 1.82 | 0.79 |
| 1:C:173:HIS:CD2 | 1:C:180:VAL:HG21 | 2.17 | 0.79 |
| 1:C:163:LEU:HD11 | 1:C:424:GLU:HG3 | 1.63 | 0.79 |
| 1:C:81:LYS:HD3 | 1:C:84:PHE:CD2 | 2.17 | 0.79 |
| 1:C:92:LEU:HD13 | 1:C:520:ASN:CA | 2.13 | 0.79 |
| 1:B:103:PHE:HD1 | 1:B:371:TRP:HB3 | 1.46 | 0.79 |
| 1:B:106:PHE:CD1 | 1:B:534:ILE:HD12 | 2.17 | 0.79 |
| 1:C:205:ALA:O | 1:C:209:PHE:HB2 | 1.83 | 0.79 |
| 1:C:144:MET:CG | 1:C:388:ILE:HD13 | 2.13 | 0.79 |
| 1:B:123:GLY:HA2 | 1:B:394:ILE:HD11 | 1.65 | 0.79 |
| 1:B:366:TRP:O | 1:B:370:TYR:CD2 | 2.36 | 0.79 |
| 1:B:206:TYR:CE2 | 1:B:543:ASP:OD2 | 2.36 | 0.79 |
| 1:C:173:HIS:CD2 | 1:C:180:VAL:HG13 | 2.17 | 0.79 |
| 1:A:350:ARG:HG2 | 1:A:363:LEU:HD11 | 1.66 | 0.79 |
| 1:B:475:VAL:O | 1:B:479:MET:HG2 | 1.83 | 0.79 |
| 1:A:574:ARG:N | 1:A:574:ARG:HD2 | 1.98 | 0.78 |
| 1:C:292:PHE:O | 1:C:296:SER:HB3 | 1.83 | 0.78 |
| 1:A:261:ILE:HD11 | 1:A:461:LEU:HD21 | 1.65 | 0.78 |
| 1:B:200:VAL:HG21 | 1:B:378:SER:CB | 2.01 | 0.78 |
| 1:A:64:VAL:CG2 | 1:A:65:PRO:HD3 | 2.14 | 0.78 |
| 1:B:128:GLY:HA2 | 1:B:209:PHE:O | 1.84 | 0.78 |
| 1:A:327:VAL:HG11 | 1:B:97:ASP:O | 1.82 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:215:GLN:HE22 | 1:C:387:ARG:HE | 1.28 | 0.78 |
| 1:B:320:VAL:CG2 | 1:B:415:ILE:HG21 | 2.13 | 0.78 |
| 1:A:156:PHE:CE1 | 1:A:157:TYR:CG | 2.72 | 0.78 |
| 1:A:285:VAL:HA | 1:A:288:LEU:HG | 1.66 | 0.78 |
| 1:A:422:VAL:HA | 1:A:425:GLN:HG3 | 1.65 | 0.78 |
| 1:B:114:ILE:HA | 1:B:117:ILE:CG2 | 2.13 | 0.78 |
| 1:A:59:ASN:OD1 | 1:A:482:HIS:CD2 | 2.36 | 0.78 |
| 1:A:295:ILE:HD13 | 1:A:492:THR:HG21 | 1.64 | 0.78 |
| 1:B:380:PHE:CE1 | 1:B:384:PHE:CE1 | 2.72 | 0.78 |
| 1:A:202:LEU:HD11 | 1:A:394:ILE:HG23 | 1.66 | 0.77 |
| 1:A:251:ALA:HA | 1:A:254:LEU:HB2 | 1.66 | 0.77 |
| 1:B:201:GLY:CA | 1:B:385:LEU:HD11 | 2.12 | 0.77 |
| 1:C:269:ASN:O | 1:C:270:ILE:HG13 | 1.84 | 0.77 |
| 1:C:134:PRO:CD | 1:C:391:GLY:O | 2.32 | 0.77 |
| 1:C:264:GLY:HA3 | 1:C:441:PHE:CE1 | 2.19 | 0.77 |
| 1:B:309:ASN:ND2 | 1:B:464:PHE:CD2 | 2.30 | 0.77 |
| 1:C:363:LEU:HD23 | 1:C:367:THR:HG21 | 1.62 | 0.77 |
| 1:C:76:TRP:HD1 | 1:C:77:GLY:N | 1.83 | 0.77 |
| 1:A:123:GLY:CA | 1:A:394:ILE:HB | 2.14 | 0.77 |
| 1:A:412:TRP:CZ2 | 1:A:416:PHE:CZ | 2.72 | 0.77 |
| 1:B:457:ALA:HA | 1:B:460:LEU:HD12 | 1.66 | 0.77 |
| 1:C:562:ARG:HA | 1:C:565:ARG:HD2 | 1.67 | 0.77 |
| 1:B:129:ARG:N | 1:B:390:ARG:HH12 | 1.82 | 0.76 |
| 1:A:92:LEU:HD23 | 1:A:520:ASN:OD1 | 1.86 | 0.76 |
| 1:A:156:PHE:HE1 | 1:A:157:TYR:CD2 | 2.03 | 0.76 |
| 1:B:127:LEU:HD11 | 1:B:205:ALA:HB1 | 1.67 | 0.76 |
| 1:B:379:PRO:HG3 | 1:B:529:PHE:CZ | 2.20 | 0.76 |
| 1:C:59:ASN:O | 1:C:63:ILE:HG13 | 1.84 | 0.76 |
| 1:B:259:LEU:HD12 | 1:B:260:GLN:N | 2.01 | 0.76 |
| 1:B:453:MET:HE3 | 1:B:456:ILE:HD11 | 1.67 | 0.76 |
| 1:C:260:GLN:OE1 | 1:C:461:LEU:HD21 | 1.86 | 0.76 |
| 1:C:304:TYR:CD1 | 1:C:305:LEU:HG | 2.20 | 0.76 |
| 1:C:471:SER:O | 1:C:475:VAL:HG23 | 1.85 | 0.76 |
| 1:C:76:TRP:CD1 | 1:C:77:GLY:N | 2.53 | 0.76 |
| 1:B:380:PHE:HE1 | 1:B:384:PHE:CE1 | 2.03 | 0.76 |
| 1:B:92:LEU:HD13 | 1:B:524:VAL:HG13 | 1.66 | 0.76 |
| 1:A:345:PHE:CE1 | 1:C:341:LEU:HD13 | 2.21 | 0.76 |
| 1:B:121:LYS:HZ1 | 1:B:550:TYR:HD1 | 1.32 | 0.76 |
| 1:B:152:ILE:HB | 1:B:464:PHE:HE1 | 1.50 | 0.76 |
| 1:B:366:TRP:CD1 | 1:B:366:TRP:N | 2.53 | 0.76 |
| 1:C:312:LEU:H | 1:C:312:LEU:HD12 | 1.49 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:370:TYR:O | 1:B:374:TRP:HD1 | 1.69 | 0.76 |
| 1:B:329:ILE:CD1 | 1:B:415:ILE:HG23 | 2.15 | 0.76 |
| 1:C:559:PHE:HA | 1:C:562:ARG:HG2 | 1.67 | 0.75 |
| 1:C:363:LEU:HA | 1:C:367:THR:CG2 | 2.17 | 0.75 |
| 1:B:114:ILE:O | 1:B:117:ILE:CG2 | 2.33 | 0.75 |
| 1:A:92:LEU:HD13 | 1:A:96:VAL:HG21 | 1.67 | 0.75 |
| 1:B:211:VAL:HG11 | 1:B:213:ARG:NE | 2.01 | 0.75 |
| 1:A:527:THR:N | 1:A:528:PRO:CD | 2.49 | 0.75 |
| 1:B:329:ILE:HD13 | 1:B:415:ILE:HG23 | 1.69 | 0.75 |
| 1:C:231:GLU:O | 1:C:236:LYS:HG2 | 1.87 | 0.75 |
| 1:C:363:LEU:O | 1:C:368:ILE:HG22 | 1.87 | 0.75 |
| 1:C:76:TRP:NE1 | 1:C:85:THR:CA | 2.47 | 0.75 |
| 1:B:208:THR:CG2 | 1:B:213:ARG:O | 2.25 | 0.75 |
| 1:C:108:THR:CA | 1:C:192:HIS:HE1 | 1.99 | 0.74 |
| 1:B:128:GLY:HA2 | 1:B:209:PHE:C | 2.08 | 0.74 |
| 1:B:452:ILE:O | 1:B:455:ILE:HG12 | 1.87 | 0.74 |
| 1:C:247:VAL:HG11 | 1:C:502:ILE:HD13 | 1.69 | 0.74 |
| 1:C:193:PRO:HB3 | 1:C:374:TRP:CD1 | 2.21 | 0.74 |
| 1:C:308:ALA:O | 1:C:312:LEU:HD13 | 1.87 | 0.74 |
| 1:A:329:ILE:HG21 | 1:A:415:ILE:HG22 | 1.69 | 0.74 |
| 1:C:224:LEU:HD11 | 1:C:539:ALA:HA | 1.70 | 0.74 |
| 1:A:329:ILE:HD11 | 1:A:419:THR:HG22 | 1.70 | 0.74 |
| 1:A:81:LYS:CB | 1:A:84:PHE:HB2 | 2.17 | 0.74 |
| 1:B:404:VAL:O | 1:B:408:VAL:HG22 | 1.88 | 0.74 |
| 1:A:295:ILE:HD11 | 1:A:470:ASP:HA | 1.69 | 0.74 |
| 1:B:161:GLU:HB3 | 1:B:162:PRO:HD3 | 1.70 | 0.74 |
| 1:B:300:LYS:O | 1:B:300:LYS:HG2 | 1.87 | 0.74 |
| 1:C:64:VAL:CG1 | 1:C:65:PRO:CD | 2.58 | 0.74 |
| 1:B:327:VAL:CG2 | 1:B:328:SER:H | 1.99 | 0.74 |
| 1:B:96:VAL:HG13 | 1:B:368:ILE:HG21 | 1.67 | 0.74 |
| 1:C:231:GLU:HG3 | 1:C:236:LYS:HE2 | 1.70 | 0.74 |
| 1:B:401:VAL:O | 1:B:405:PRO:HG2 | 1.88 | 0.74 |
| 1:B:527:THR:HB | 1:B:528:PRO:HD3 | 1.70 | 0.74 |
| 1:B:64:VAL:HB | 1:B:65:PRO:HD3 | 1.68 | 0.74 |
| 1:A:309:ASN:OD1 | 1:A:464:PHE:CE1 | 2.41 | 0.74 |
| 1:C:120:SER:OG | 1:C:122:PHE:HD2 | 1.69 | 0.74 |
| 1:A:301:GLY:O | 1:A:302:ILE:HG12 | 1.88 | 0.73 |
| 1:A:530:LEU:O | 1:A:534:ILE:HG12 | 1.88 | 0.73 |
| 1:B:92:LEU:HD11 | 1:B:523:ILE:CB | 2.13 | 0.73 |
| 1:C:108:THR:HA | 1:C:192:HIS:HE1 | 1.49 | 0.73 |
| 1:C:134:PRO:HG3 | 1:C:392:ARG:HD3 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:264:GLY:HA3 | 1:C:441:PHE:CZ | 2.23 | 0.73 |
| 1:A:68:VAL:O | 1:A:72:ALA:HB2 | 1.88 | 0.73 |
| 1:C:288:LEU:O | 1:C:291:ILE:HG22 | 1.88 | 0.73 |
| 1:B:92:LEU:O | 1:B:95:VAL:HG12 | 1.88 | 0.73 |
| 1:C:124:THR:HG23 | 1:C:395:ARG:HH21 | 1.51 | 0.73 |
| 1:C:61:SER:O | 1:C:65:PRO:CG | 2.36 | 0.73 |
| 1:A:527:THR:CG2 | 1:A:528:PRO:HD3 | 2.18 | 0.73 |
| 1:B:186:MET:HG2 | 1:B:190:THR:CG2 | 2.19 | 0.73 |
| 1:B:121:LYS:NZ | 1:B:550:TYR:HD1 | 1.86 | 0.73 |
| 1:B:142:ILE:HA | 1:B:145:MET:SD | 2.27 | 0.73 |
| 1:B:237:LEU:O | 1:B:241:LEU:HG | 1.89 | 0.73 |
| 1:B:128:GLY:HA3 | 1:B:390:ARG:NH1 | 2.03 | 0.73 |
| 1:C:144:MET:SD | 1:C:388:ILE:HG12 | 2.29 | 0.73 |
| 1:B:346:GLN:HG3 | 1:B:347:MET:N | 2.04 | 0.73 |
| 1:B:316:LEU:HD22 | 1:B:460:LEU:HD12 | 1.70 | 0.73 |
| 1:C:209:PHE:CE1 | 1:C:390:ARG:HB2 | 2.24 | 0.73 |
| 1:A:302:ILE:CG1 | 1:A:303:GLN:H | 2.00 | 0.73 |
| 1:A:309:ASN:OD1 | 1:A:464:PHE:HE1 | 1.70 | 0.73 |
| 1:B:470:ASP:O | 1:B:474:THR:HG23 | 1.89 | 0.73 |
| 1:B:539:ALA:O | 1:B:543:ASP:HB3 | 1.88 | 0.73 |
| 1:C:144:MET:SD | 1:C:388:ILE:CD1 | 2.77 | 0.73 |
| 1:A:112:PHE:O | 1:A:116:VAL:CG1 | 2.36 | 0.72 |
| 1:B:175:GLU:O | 1:B:176:HIS:HB2 | 1.87 | 0.72 |
| 1:B:197:TYR:HH | 1:B:374:TRP:HE3 | 1.36 | 0.72 |
| 1:C:248:PHE:HB3 | 1:C:522:THR:HG22 | 1.70 | 0.72 |
| 1:B:104:ILE:HD12 | 1:B:105:LEU:N | 2.04 | 0.72 |
| 1:B:456:ILE:O | 1:B:460:LEU:HG | 1.88 | 0.72 |
| 1:C:264:GLY:CA | 1:C:441:PHE:CZ | 2.72 | 0.72 |
| 1:C:76:TRP:CE2 | 1:C:85:THR:HA | 2.23 | 0.72 |
| 1:A:66:ALA:O | 1:A:70:VAL:HG23 | 1.89 | 0.72 |
| 1:A:183:SER:OG | 1:A:339:ASN:HB3 | 1.88 | 0.72 |
| 1:C:134:PRO:CG | 1:C:391:GLY:O | 2.37 | 0.72 |
| 1:B:95:VAL:HG21 | 1:B:527:THR:HG21 | 1.70 | 0.72 |
| 1:A:197:TYR:CE1 | 1:A:381:VAL:HG21 | 2.25 | 0.72 |
| 1:B:78:ILE:CG2 | 1:B:79:GLY:H | 2.02 | 0.72 |
| 1:C:122:PHE:CD1 | 1:C:544:LEU:HB3 | 2.25 | 0.72 |
| 1:C:416:PHE:CE1 | 1:C:440:LEU:HD11 | 2.25 | 0.72 |
| 1:B:135:GLU:HG2 | 1:B:136:PHE:CD2 | 2.25 | 0.71 |
| 1:C:230:ALA:O | 1:C:231:GLU:CB | 2.38 | 0.71 |
| 1:A:387:ARG:HH11 | 1:A:387:ARG:HB3 | 1.54 | 0.71 |
| 1:A:154:LEU:O | 1:A:158:GLY:HA3 | 1.90 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:312:LEU:CB | 1:B:460:LEU:HD21 | 2.07 | 0.71 |
| 1:C:108:THR:CA | 1:C:192:HIS:CE1 | 2.72 | 0.71 |
| 1:C:148:ALA:HB2 | 1:C:384:PHE:CE2 | 2.26 | 0.71 |
| 1:A:161:GLU:HG3 | 1:A:366:TRP:HZ3 | 1.56 | 0.71 |
| 1:B:343:ASN:O | 1:B:347:MET:CG | 2.36 | 0.71 |
| 1:B:110:PHE:CD1 | 1:B:196:ILE:CG2 | 2.73 | 0.71 |
| 1:C:76:TRP:C | 1:C:76:TRP:CD1 | 2.63 | 0.71 |
| 1:A:106:PHE:HB3 | 1:A:534:ILE:HD11 | 1.73 | 0.70 |
| 1:A:245:ALA:HB2 | 1:A:526:ALA:HB2 | 1.73 | 0.70 |
| 1:A:72:ALA:O | 1:A:76:TRP:HB2 | 1.91 | 0.70 |
| 1:B:110:PHE:HD1 | 1:B:196:ILE:CG2 | 2.04 | 0.70 |
| 1:B:283:VAL:HA | 1:B:286:LEU:HG | 1.71 | 0.70 |
| 1:B:464:PHE:O | 1:B:468:SER:N | 2.23 | 0.70 |
| 1:C:305:LEU:HA | 1:C:308:ALA:HB3 | 1.73 | 0.70 |
| 1:A:302:ILE:HG13 | 1:A:303:GLN:H | 1.54 | 0.70 |
| 1:A:329:ILE:HG23 | 1:A:414:SER:O | 1.91 | 0.70 |
| 1:B:177:ASN:HD21 | 1:B:180:VAL:HG23 | 1.56 | 0.70 |
| 1:C:224:LEU:CD1 | 1:C:539:ALA:HB2 | 2.20 | 0.70 |
| 1:B:365:SER:CB | 1:B:366:TRP:CD1 | 2.73 | 0.70 |
| 1:A:235:GLY:H | 1:A:238:ILE:HD13 | 1.56 | 0.70 |
| 1:B:476:MET:HB3 | 1:B:495:TRP:CE3 | 2.27 | 0.70 |
| 1:C:281:GLY:O | 1:C:285:VAL:HG22 | 1.91 | 0.70 |
| 1:C:379:PRO:HD3 | 1:C:529:PHE:CE2 | 2.26 | 0.70 |
| 1:A:209:PHE:CE2 | 1:A:390:ARG:HG2 | 2.26 | 0.70 |
| 1:C:414:SER:O | 1:C:418:GLY:HA3 | 1.90 | 0.70 |
| 1:C:456:ILE:O | 1:C:459:ILE:HG22 | 1.90 | 0.70 |
| 1:B:451:GLN:H | 1:B:451:GLN:CD | 1.95 | 0.70 |
| 1:C:303:GLN:O | 1:C:304:TYR:HB3 | 1.92 | 0.70 |
| 1:B:114:ILE:HD12 | 1:B:402:LEU:HD21 | 1.74 | 0.70 |
| 1:A:353:MET:HE2 | 1:A:353:MET:HA | 1.72 | 0.69 |
| 1:B:92:LEU:HD12 | 1:B:524:VAL:HG13 | 1.74 | 0.69 |
| 1:B:95:VAL:HG21 | 1:B:527:THR:HG23 | 1.74 | 0.69 |
| 1:C:389:SER:O | 1:C:390:ARG:C | 2.30 | 0.69 |
| 1:A:412:TRP:CD2 | 1:A:416:PHE:HE2 | 2.09 | 0.69 |
| 1:A:63:ILE:O | 1:A:66:ALA:HB3 | 1.93 | 0.69 |
| 1:B:435:ALA:O | 1:B:438:GLU:HG2 | 1.92 | 0.69 |
| 1:A:112:PHE:O | 1:A:116:VAL:HG13 | 1.93 | 0.69 |
| 1:A:344:PHE:O | 1:A:344:PHE:CD2 | 2.44 | 0.69 |
| 1:B:270:ILE:HD12 | 1:B:270:ILE:H | 1.57 | 0.69 |
| 1:C:186:MET:HE3 | 1:C:190:THR:HG21 | 1.74 | 0.69 |
| 1:A:114:ILE:HD13 | 1:A:195:ALA:CB | 2.22 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:412:TRP:CH2 | 1:A:416:PHE:CZ | 2.81 | 0.69 |
| 1:C:134:PRO:HD3 | 1:C:391:GLY:O | 1.93 | 0.69 |
| 1:A:473:SER:HA | 1:A:476:MET:HG2 | 1.75 | 0.69 |
| 1:B:225:ILE:HG21 | 1:B:230:ALA:HA | 1.73 | 0.69 |
| 1:C:401:VAL:O | 1:C:405:PRO:HD2 | 1.91 | 0.69 |
| 1:A:101:TRP:CZ2 | 1:C:330:LEU:HD13 | 2.27 | 0.69 |
| 1:A:444:LEU:CD1 | 1:A:450:GLY:O | 2.41 | 0.69 |
| 1:B:189:TRP:CH2 | 1:B:370:TYR:OH | 2.44 | 0.69 |
| 1:C:76:TRP:CZ2 | 1:C:85:THR:HA | 2.28 | 0.69 |
| 1:A:309:ASN:CG | 1:A:464:PHE:CE1 | 2.62 | 0.69 |
| 1:B:464:PHE:HA | 1:B:467:THR:CG2 | 2.22 | 0.68 |
| 1:A:222:VAL:HA | 1:A:226:GLY:O | 1.93 | 0.68 |
| 1:C:416:PHE:HE1 | 1:C:440:LEU:HD11 | 1.58 | 0.68 |
| 1:B:320:VAL:HG11 | 1:B:416:PHE:CE1 | 2.28 | 0.68 |
| 1:C:64:VAL:O | 1:C:68:VAL:HG23 | 1.93 | 0.68 |
| 1:C:354:SER:O | 1:C:359:ALA:HB3 | 1.93 | 0.68 |
| 1:C:224:LEU:CD1 | 1:C:539:ALA:CA | 2.67 | 0.68 |
| 1:C:66:ALA:N | 1:C:240:ILE:HD11 | 2.09 | 0.68 |
| 1:A:369:PHE:CE1 | 1:A:519:GLN:CB | 2.65 | 0.68 |
| 1:B:177:ASN:OD1 | 1:B:177:ASN:C | 2.30 | 0.68 |
| 1:B:369:PHE:HA | 1:B:523:ILE:HD12 | 1.76 | 0.68 |
| 1:A:243:ILE:HD12 | 1:A:244:ILE:N | 2.09 | 0.68 |
| 1:B:540:LEU:O | 1:B:544:LEU:HG | 1.93 | 0.68 |
| 1:C:121:LYS:N | 1:C:121:LYS:HD3 | 2.05 | 0.68 |
| 1:A:412:TRP:CD2 | 1:A:416:PHE:CE2 | 2.82 | 0.68 |
| 1:A:114:ILE:HD13 | 1:A:195:ALA:HB1 | 1.76 | 0.68 |
| 1:A:379:PRO:HG3 | 1:A:529:PHE:CE2 | 2.29 | 0.68 |
| 1:A:309:ASN:ND2 | 1:A:464:PHE:HE1 | 1.91 | 0.68 |
| 1:C:103:PHE:CE2 | 1:C:530:LEU:HD23 | 2.28 | 0.68 |
| 1:C:520:ASN:O | 1:C:524:VAL:HG23 | 1.93 | 0.67 |
| 1:A:412:TRP:CH2 | 1:A:416:PHE:CE2 | 2.81 | 0.67 |
| 1:A:199:ILE:HG22 | 1:A:536:LEU:HD23 | 1.76 | 0.67 |
| 1:B:373:TRP:HD1 | 1:B:373:TRP:C | 1.97 | 0.67 |
| 1:C:506:LEU:HD23 | 1:C:518:LEU:HD12 | 1.74 | 0.67 |
| 1:A:404:VAL:O | 1:A:408:VAL:HG13 | 1.94 | 0.67 |
| 1:A:327:VAL:HG21 | 1:B:98:ASN:OD1 | 1.94 | 0.67 |
| 1:C:156:PHE:CE1 | 1:C:256:LEU:HB2 | 2.29 | 0.67 |
| 1:C:270:ILE:HA | 1:C:271:ILE:HG12 | 1.75 | 0.67 |
| 1:C:371:TRP:N | 1:C:371:TRP:HE3 | 1.91 | 0.67 |
| 1:B:213:ARG:NH1 | 1:B:222:VAL:HB | 2.10 | 0.67 |
| 1:B:398:ILE:O | 1:B:402:LEU:CD1 | 2.35 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:76:TRP:NE1 | 1:C:85:THR:CB | 2.54 | 0.67 |
| 1:A:476:MET:SD | 1:A:495:TRP:HB3 | 2.35 | 0.67 |
| 1:C:304:TYR:CE1 | 1:C:305:LEU:CG | 2.76 | 0.67 |
| 1:B:186:MET:CE | 1:B:336:SER:HB3 | 2.25 | 0.67 |
| 1:A:71:LEU:HA | 1:A:74:VAL:HB | 1.77 | 0.67 |
| 1:A:351:THR:HG22 | 1:C:331:ASN:HB3 | 1.76 | 0.67 |
| 1:C:134:PRO:CA | 1:C:391:GLY:HA3 | 2.18 | 0.67 |
| 1:A:478:THR:HA | 1:A:481:GLN:HE21 | 1.60 | 0.67 |
| 1:C:329:ILE:CG2 | 1:C:415:ILE:HG12 | 2.25 | 0.67 |
| 1:C:103:PHE:CD2 | 1:C:530:LEU:CD2 | 2.76 | 0.67 |
| 1:A:158:GLY:HA2 | 1:A:413:PHE:HE1 | 1.60 | 0.66 |
| 1:C:193:PRO:HB3 | 1:C:374:TRP:NE1 | 2.11 | 0.66 |
| 1:C:433:ASP:OD1 | 1:C:433:ASP:C | 2.31 | 0.66 |
| 1:C:230:ALA:O | 1:C:231:GLU:HB3 | 1.95 | 0.66 |
| 1:C:431:TRP:NE1 | 1:C:434:GLY:HA2 | 2.09 | 0.66 |
| 1:B:423:PHE:HB3 | 1:B:428:GLU:O | 1.95 | 0.66 |
| 1:C:264:GLY:CA | 1:C:441:PHE:CE1 | 2.77 | 0.66 |
| 1:C:389:SER:OG | 1:C:397:PHE:CD1 | 2.48 | 0.66 |
| 1:B:327:VAL:O | 1:B:331:ASN:N | 2.29 | 0.66 |
| 1:C:95:VAL:HG21 | 1:C:527:THR:CG2 | 2.25 | 0.66 |
| 1:C:163:LEU:CG | 1:C:431:TRP:HZ3 | 2.04 | 0.66 |
| 1:C:561:ALA:O | 1:C:565:ARG:HG3 | 1.94 | 0.66 |
| 1:A:136:PHE:HE2 | 1:A:388:ILE:HG23 | 1.59 | 0.66 |
| 1:B:341:LEU:HB3 | 1:C:345:PHE:CD2 | 2.30 | 0.66 |
| 1:C:473:SER:HA | 1:C:476:MET:HE2 | 1.78 | 0.66 |
| 1:B:158:GLY:HA2 | 1:B:413:PHE:HE1 | 1.54 | 0.66 |
| 1:B:329:ILE:HG21 | 1:B:415:ILE:HG13 | 1.77 | 0.66 |
| 1:C:106:PHE:HA | 1:C:109:VAL:CG2 | 2.26 | 0.66 |
| 1:C:144:MET:CB | 1:C:388:ILE:HD13 | 2.26 | 0.66 |
| 1:C:67:LEU:O | 1:C:70:VAL:HG12 | 1.94 | 0.66 |
| 1:A:137:ARG:HD3 | 1:A:138:THR:N | 2.10 | 0.66 |
| 1:C:208:THR:HG21 | 1:C:215:GLN:HG3 | 1.78 | 0.66 |
| 1:C:164:THR:HG21 | 1:C:366:TRP:HZ2 | 1.60 | 0.66 |
| 1:C:194:TRP:HZ3 | 1:C:385:LEU:HD11 | 1.61 | 0.66 |
| 1:C:253:SER:OG | 1:C:377:TRP:CH2 | 2.47 | 0.66 |
| 1:B:384:PHE:CZ | 1:B:471:SER:HB2 | 2.31 | 0.66 |
| 1:B:79:GLY:O | 1:B:80:PHE:HB3 | 1.96 | 0.66 |
| 1:C:353:MET:O | 1:C:357:GLY:N | 2.29 | 0.66 |
| 1:C:76:TRP:HZ2 | 1:C:84:PHE:O | 1.79 | 0.66 |
| 1:A:449:GLY:O | 1:A:452:ILE:HG12 | 1.95 | 0.65 |
| 1:B:59:ASN:HB3 | 1:B:480:SER:O | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:192:HIS:N | 1:C:193:PRO:CD | 2.59 | 0.65 |
| 1:B:200:VAL:HG12 | 1:B:382:GLY:HA3 | 1.79 | 0.65 |
| 1:B:372:ALA:HB3 | 1:B:523:ILE:HG23 | 1.77 | 0.65 |
| 1:A:152:ILE:H | 1:A:152:ILE:HD12 | 1.61 | 0.65 |
| 1:B:279:ILE:HA | 1:B:282:ILE:HG23 | 1.78 | 0.65 |
| 1:B:305:LEU:HB3 | 1:B:467:THR:CG2 | 2.27 | 0.65 |
| 1:A:113:PHE:CZ | 1:A:117:ILE:HD12 | 2.31 | 0.65 |
| 1:A:92:LEU:O | 1:A:95:VAL:CG2 | 2.44 | 0.65 |
| 1:C:225:ILE:HG22 | 1:C:226:GLY:O | 1.96 | 0.65 |
| 1:C:226:GLY:CA | 1:C:227:GLU:HB2 | 2.17 | 0.65 |
| 1:B:157:TYR:HA | 1:B:160:THR:HG22 | 1.79 | 0.65 |
| 1:B:117:ILE:HG23 | 1:B:398:ILE:CD1 | 2.27 | 0.64 |
| 1:A:150:MET:SD | 1:A:309:ASN:HB3 | 2.36 | 0.64 |
| 1:B:185:THR:O | 1:B:189:TRP:HE3 | 1.80 | 0.64 |
| 1:B:404:VAL:HB | 1:B:405:PRO:HD3 | 1.79 | 0.64 |
| 1:C:173:HIS:CG | 1:C:180:VAL:HG21 | 2.32 | 0.64 |
| 1:C:426:ASN:HB2 | 1:C:428:GLU:OE1 | 1.98 | 0.64 |
| 1:A:329:ILE:HD11 | 1:A:419:THR:HG23 | 1.78 | 0.64 |
| 1:A:206:TYR:HE2 | 1:A:543:ASP:CG | 2.00 | 0.64 |
| 1:B:418:GLY:O | 1:B:422:VAL:HG23 | 1.98 | 0.64 |
| 1:C:113:PHE:CD2 | 1:C:199:ILE:HD11 | 2.32 | 0.64 |
| 1:C:312:LEU:N | 1:C:312:LEU:HD12 | 2.12 | 0.64 |
| 1:A:283:VAL:HA | 1:A:286:LEU:HD12 | 1.79 | 0.64 |
| 1:A:163:LEU:HD21 | 1:A:424:GLU:OE2 | 1.97 | 0.64 |
| 1:A:453:MET:O | 1:A:456:ILE:HG12 | 1.98 | 0.64 |
| 1:A:246:THR:O | 1:A:250:THR:HG23 | 1.97 | 0.64 |
| 1:B:291:ILE:HA | 1:B:466:ILE:CD1 | 2.27 | 0.64 |
| 1:C:404:VAL:HB | 1:C:405:PRO:HD3 | 1.78 | 0.64 |
| 1:A:222:VAL:CG2 | 1:A:227:GLU:HG2 | 2.28 | 0.64 |
| 1:A:223:PRO:CG | 1:A:543:ASP:HB2 | 2.28 | 0.64 |
| 1:B:231:GLU:HG3 | 1:B:236:LYS:HE3 | 1.80 | 0.64 |
| 1:B:267:ALA:HB1 | 1:B:445:HIS:HE1 | 1.62 | 0.64 |
| 1:C:76:TRP:HE1 | 1:C:85:THR:HB | 1.58 | 0.64 |
| 1:A:369:PHE:CZ | 1:A:519:GLN:CB | 2.74 | 0.64 |
| 1:B:208:THR:O | 1:B:212:GLY:CA | 2.41 | 0.64 |
| 1:A:295:ILE:HG21 | 1:A:492:THR:HG21 | 1.80 | 0.63 |
| 1:B:312:LEU:CB | 1:B:460:LEU:CD2 | 2.70 | 0.63 |
| 1:C:464:PHE:O | 1:C:468:SER:HB2 | 1.97 | 0.63 |
| 1:B:455:ILE:HG13 | 1:B:456:ILE:N | 2.13 | 0.63 |
| 1:C:292:PHE:O | 1:C:296:SER:N | 2.30 | 0.63 |
| 1:C:319:PHE:O | 1:C:323:VAL:HG12 | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:267:ALA:HB1 | 1:B:445:HIS:CE1 | 2.33 | 0.63 |
| 1:C:380:PHE:CD1 | 1:C:380:PHE:C | 2.70 | 0.63 |
| 1:C:503:GLY:O | 1:C:507:LEU:HD13 | 1.99 | 0.63 |
| 1:B:135:GLU:HG2 | 1:B:136:PHE:CE2 | 2.33 | 0.63 |
| 1:B:197:TYR:OH | 1:B:374:TRP:CE3 | 2.51 | 0.63 |
| 1:B:243:ILE:O | 1:B:246:THR:HG22 | 1.99 | 0.63 |
| 1:B:320:VAL:CG2 | 1:B:415:ILE:HG22 | 2.29 | 0.63 |
| 1:C:202:LEU:HD23 | 1:C:540:LEU:HD21 | 1.80 | 0.63 |
| 1:C:60:TRP:O | 1:C:64:VAL:HG12 | 1.99 | 0.63 |
| 1:B:365:SER:CB | 1:B:366:TRP:HD1 | 2.12 | 0.63 |
| 1:C:267:ALA:HB1 | 1:C:451:GLN:CD | 2.19 | 0.63 |
| 1:C:488:ASN:O | 1:C:491:VAL:HG12 | 1.99 | 0.63 |
| 1:C:95:VAL:HG21 | 1:C:527:THR:HG21 | 1.80 | 0.62 |
| 1:A:404:VAL:HB | 1:A:405:PRO:HD3 | 1.81 | 0.62 |
| 1:B:380:PHE:HE1 | 1:B:384:PHE:CZ | 2.16 | 0.62 |
| 1:C:164:THR:HG21 | 1:C:366:TRP:CZ2 | 2.34 | 0.62 |
| 1:C:371:TRP:CE3 | 1:C:371:TRP:N | 2.67 | 0.62 |
| 1:C:431:TRP:CD1 | 1:C:434:GLY:HA2 | 2.34 | 0.62 |
| 1:B:366:TRP:O | 1:B:370:TYR:HD2 | 1.80 | 0.62 |
| 1:A:318:ILE:O | 1:A:322:VAL:HG22 | 1.98 | 0.62 |
| 1:C:155:MET:HB3 | 1:C:260:GLN:HE22 | 1.64 | 0.62 |
| 1:C:267:ALA:HB1 | 1:C:451:GLN:NE2 | 2.14 | 0.62 |
| 1:A:129:ARG:NH2 | 1:A:212:GLY:HA3 | 2.14 | 0.62 |
| 1:A:579:ALA:O | 1:A:582:ARG:HG2 | 2.00 | 0.62 |
| 1:B:192:HIS:HB2 | 1:B:193:PRO:HD3 | 1.82 | 0.62 |
| 1:A:97:ASP:O | 1:C:327:VAL:HG11 | 1.99 | 0.62 |
| 1:A:378:SER:HA | 1:A:381:VAL:CG2 | 2.30 | 0.62 |
| 1:C:304:TYR:HE1 | 1:C:305:LEU:HG | 1.57 | 0.62 |
| 1:C:259:LEU:HD23 | 1:C:507:LEU:HG | 1.81 | 0.62 |
| 1:A:170:VAL:HG13 | 1:A:171:PRO:HD2 | 1.80 | 0.62 |
| 1:A:175:GLU:O | 1:A:176:HIS:HB2 | 1.99 | 0.62 |
| 1:A:323:VAL:HG12 | 1:A:447:LEU:HD22 | 1.82 | 0.62 |
| 1:A:295:ILE:HD13 | 1:A:492:THR:CG2 | 2.30 | 0.62 |
| 1:A:478:THR:O | 1:A:481:GLN:HG2 | 2.00 | 0.62 |
| 1:B:103:PHE:HB3 | 1:B:371:TRP:CD1 | 2.35 | 0.62 |
| 1:B:203:ALA:HB2 | 1:B:540:LEU:HD22 | 1.82 | 0.62 |
| 1:C:105:LEU:O | 1:C:109:VAL:CG2 | 2.40 | 0.62 |
| 1:C:279:ILE:O | 1:C:283:VAL:HG23 | 2.00 | 0.62 |
| 1:C:333:LEU:O | 1:C:337:ILE:HG12 | 1.99 | 0.62 |
| 1:C:65:PRO:O | 1:C:69:ILE:HD13 | 1.99 | 0.62 |
| 1:A:137:ARG:HH11 | 1:A:139:VAL:HG22 | 1.65 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:451:GLN:O | 1:A:455:ILE:HG13 | 2.00 | 0.61 |
| 1:B:366:TRP:N | 1:B:366:TRP:HD1 | 1.97 | 0.61 |
| 1:B:78:ILE:CG2 | 1:B:79:GLY:N | 2.57 | 0.61 |
| 1:C:188:HIS:HB3 | 1:C:370:TYR:CD2 | 2.35 | 0.61 |
| 1:A:225:ILE:O | 1:A:225:ILE:HG22 | 2.00 | 0.61 |
| 1:A:562:ARG:O | 1:A:565:ARG:HB2 | 2.00 | 0.61 |
| 1:B:144:MET:HB2 | 1:B:388:ILE:HD11 | 1.82 | 0.61 |
| 1:B:365:SER:C | 1:B:366:TRP:CD1 | 2.74 | 0.61 |
| 1:B:323:VAL:HG23 | 1:B:447:LEU:HD22 | 1.82 | 0.61 |
| 1:A:490:TRP:CD1 | 1:A:491:VAL:HG13 | 2.31 | 0.61 |
| 1:B:172:GLY:O | 1:B:173:HIS:CD2 | 2.54 | 0.61 |
| 1:B:533:VAL:O | 1:B:536:LEU:HB3 | 2.01 | 0.61 |
| 1:C:473:SER:HB3 | 1:C:492:THR:O | 2.00 | 0.61 |
| 1:A:122:PHE:HE1 | 1:A:545:SER:HA | 1.66 | 0.61 |
| 1:B:194:TRP:CE2 | 1:B:405:PRO:HB3 | 2.36 | 0.61 |
| 1:B:282:ILE:O | 1:B:285:VAL:HG12 | 2.01 | 0.61 |
| 1:A:223:PRO:HG2 | 1:A:543:ASP:HB2 | 1.82 | 0.61 |
| 1:A:170:VAL:HG22 | 1:A:362:TRP:CZ2 | 2.36 | 0.61 |
| 1:A:392:ARG:HD2 | 1:A:396:GLU:HG3 | 1.83 | 0.61 |
| 1:A:481:GLN:O | 1:A:482:HIS:CB | 2.41 | 0.61 |
| 1:C:88:ALA:O | 1:C:91:ALA:HB3 | 2.01 | 0.61 |
| 1:A:167:ARG:HG2 | 1:A:168:ASN:OD1 | 2.00 | 0.61 |
| 1:B:223:PRO:HG3 | 1:B:543:ASP:HB2 | 1.83 | 0.61 |
| 1:B:372:ALA:HB2 | 1:B:523:ILE:HG23 | 1.83 | 0.61 |
| 1:A:97:ASP:O | 1:C:327:VAL:CG1 | 2.48 | 0.61 |
| 1:B:476:MET:HB3 | 1:B:495:TRP:HE3 | 1.64 | 0.60 |
| 1:A:327:VAL:CG1 | 1:B:97:ASP:O | 2.46 | 0.60 |
| 1:C:165:PHE:CE1 | 1:C:362:TRP:HZ2 | 2.19 | 0.60 |
| 1:B:110:PHE:CE1 | 1:B:196:ILE:HG22 | 2.35 | 0.60 |
| 1:B:365:SER:HB2 | 1:B:366:TRP:CD1 | 2.36 | 0.60 |
| 1:B:375:ILE:HG23 | 1:B:526:ALA:HB1 | 1.82 | 0.60 |
| 1:A:64:VAL:HG23 | 1:A:65:PRO:CD | 2.28 | 0.60 |
| 1:C:325:PRO:O | 1:C:329:ILE:HG13 | 2.01 | 0.60 |
| 1:C:375:ILE:HD12 | 1:C:530:LEU:HB2 | 1.83 | 0.60 |
| 1:C:488:ASN:HB3 | 1:C:491:VAL:HG12 | 1.83 | 0.60 |
| 1:C:524:VAL:HA | 1:C:527:THR:HG23 | 1.84 | 0.60 |
| 1:A:311:VAL:O | 1:A:315:LEU:HB2 | 2.02 | 0.60 |
| 1:B:312:LEU:HD13 | 1:B:460:LEU:HD23 | 1.82 | 0.60 |
| 1:C:148:ALA:C | 2:C:2486:CHT:H62 | 2.18 | 0.60 |
| 1:C:375:ILE:HD13 | 1:C:530:LEU:CA | 2.23 | 0.60 |
| 1:A:222:VAL:HB | 1:A:227:GLU:HG2 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:144:MET:HB3 | 1:C:388:ILE:HD13 | 1.84 | 0.60 |
| 1:C:163:LEU:CD1 | 1:C:424:GLU:HG3 | 2.31 | 0.60 |
| 1:A:369:PHE:HZ | 1:A:519:GLN:HB2 | 1.60 | 0.60 |
| 1:B:186:MET:HE1 | 1:B:336:SER:HB3 | 1.83 | 0.60 |
| 1:B:197:TYR:OH | 1:B:374:TRP:HE3 | 1.84 | 0.60 |
| 1:B:417:GLY:O | 1:B:421:ILE:HG12 | 2.02 | 0.60 |
| 1:C:152:ILE:HG12 | 1:C:464:PHE:HB3 | 1.84 | 0.60 |
| 1:A:215:GLN:CD | 1:A:387:ARG:NH2 | 2.54 | 0.60 |
| 1:A:243:ILE:HD12 | 1:A:244:ILE:HG13 | 1.84 | 0.60 |
| 1:A:309:ASN:O | 1:A:313:ALA:HB3 | 2.01 | 0.60 |
| 1:A:88:ALA:HA | 1:A:91:ALA:HB3 | 1.84 | 0.60 |
| 1:C:91:ALA:O | 1:C:94:ALA:CB | 2.46 | 0.60 |
| 1:A:149:GLY:HA2 | 1:A:194:TRP:HH2 | 1.66 | 0.60 |
| 1:B:365:SER:HB2 | 1:B:366:TRP:HD1 | 1.67 | 0.60 |
| 1:B:114:ILE:CD1 | 1:B:402:LEU:HD21 | 2.32 | 0.60 |
| 1:C:230:ALA:O | 1:C:231:GLU:CG | 2.49 | 0.60 |
| 1:C:375:ILE:CD1 | 1:C:530:LEU:HA | 2.25 | 0.60 |
| 1:A:161:GLU:HG3 | 1:A:366:TRP:CZ3 | 2.34 | 0.60 |
| 1:B:208:THR:HG1 | 1:B:209:PHE:HD1 | 1.50 | 0.60 |
| 1:B:411:VAL:CG1 | 1:B:415:ILE:CD1 | 2.76 | 0.60 |
| 1:B:453:MET:CE | 1:B:456:ILE:HD11 | 2.31 | 0.60 |
| 1:C:114:ILE:CG1 | 1:C:398:ILE:HG12 | 2.32 | 0.60 |
| 1:A:412:TRP:CE3 | 1:A:416:PHE:HE2 | 2.20 | 0.60 |
| 1:C:114:ILE:CD1 | 1:C:117:ILE:HD11 | 2.29 | 0.60 |
| 1:A:329:ILE:HG21 | 1:A:415:ILE:CG2 | 2.31 | 0.59 |
| 1:B:321:PHE:HA | 1:B:329:ILE:HD12 | 1.84 | 0.59 |
| 1:C:454:GLY:O | 1:C:457:ALA:HB3 | 2.01 | 0.59 |
| 1:A:380:PHE:HA | 1:A:475:VAL:HG11 | 1.85 | 0.59 |
| 1:B:117:ILE:HG23 | 1:B:118:ALA:N | 2.17 | 0.59 |
| 1:B:123:GLY:HA2 | 1:B:394:ILE:CD1 | 2.31 | 0.59 |
| 1:C:128:GLY:HA2 | 1:C:209:PHE:O | 2.02 | 0.59 |
| 1:C:312:LEU:H | 1:C:312:LEU:CD1 | 2.14 | 0.59 |
| 1:C:78:ILE:HG13 | 1:C:79:GLY:N | 2.17 | 0.59 |
| 1:C:161:GLU:HG3 | 1:C:185:THR:HG22 | 1.83 | 0.59 |
| 1:C:188:HIS:CB | 1:C:370:TYR:CD2 | 2.85 | 0.59 |
| 1:C:380:PHE:CE2 | 2:C:2486:CHT:H82 | 2.38 | 0.59 |
| 1:A:331:ASN:OD1 | 1:B:101:TRP:HB3 | 2.02 | 0.59 |
| 1:A:463:THR:O | 1:A:466:ILE:HG13 | 2.02 | 0.59 |
| 1:C:323:VAL:HG13 | 1:C:324:GLY:N | 2.16 | 0.59 |
| 1:B:100:GLY:O | 1:B:104:ILE:HG13 | 2.02 | 0.59 |
| 1:B:167:ARG:HH11 | 1:B:424:GLU:CD | 2.05 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:113:PHE:CZ | 1:A:117:ILE:CD1 | 2.85 | 0.59 |
| 1:A:166:TYR:CE2 | 1:A:176:HIS:CD2 | 2.90 | 0.59 |
| 1:A:550:TYR:CE1 | 1:A:554:ARG:NH1 | 2.71 | 0.59 |
| 1:B:463:THR:O | 1:B:464:PHE:CG | 2.56 | 0.59 |
| 1:C:65:PRO:HB2 | 1:C:240:ILE:CD1 | 2.33 | 0.59 |
| 1:A:101:TRP:CG | 1:A:102:ALA:N | 2.71 | 0.59 |
| 1:A:370:TYR:HB3 | 1:A:374:TRP:NE1 | 2.18 | 0.59 |
| 1:C:432:GLY:O | 1:C:433:ASP:CG | 2.41 | 0.59 |
| 1:A:388:ILE:O | 1:A:388:ILE:HG22 | 2.02 | 0.59 |
| 1:B:463:THR:HG23 | 1:B:464:PHE:CD2 | 2.37 | 0.59 |
| 1:C:363:LEU:CA | 1:C:367:THR:HG22 | 2.26 | 0.59 |
| 1:A:484:GLN:HB2 | 1:A:486:GLU:OE1 | 2.02 | 0.59 |
| 1:A:542:LYS:O | 1:A:545:SER:OG | 2.20 | 0.59 |
| 1:B:401:VAL:O | 1:B:401:VAL:HG22 | 2.03 | 0.59 |
| 1:B:74:VAL:O | 1:B:78:ILE:CG1 | 2.49 | 0.59 |
| 1:A:379:PRO:HG3 | 1:A:529:PHE:CZ | 2.38 | 0.58 |
| 1:B:257:GLY:O | 1:B:261:ILE:HG12 | 2.03 | 0.58 |
| 1:C:106:PHE:HA | 1:C:109:VAL:HG23 | 1.85 | 0.58 |
| 1:C:159:THR:HA | 1:C:417:GLY:HA2 | 1.85 | 0.58 |
| 1:A:222:VAL:CA | 1:A:226:GLY:O | 2.50 | 0.58 |
| 1:B:202:LEU:HD23 | 1:B:540:LEU:HD21 | 1.84 | 0.58 |
| 1:B:365:SER:HB3 | 1:B:366:TRP:CD1 | 2.37 | 0.58 |
| 1:B:372:ALA:HB1 | 1:B:523:ILE:HA | 1.85 | 0.58 |
| 1:B:75:VAL:O | 1:B:78:ILE:N | 2.35 | 0.58 |
| 1:C:184:THR:O | 1:C:187:PHE:HB3 | 2.03 | 0.58 |
| 1:C:481:GLN:O | 1:C:482:HIS:HB2 | 2.03 | 0.58 |
| 1:B:207:SER:O | 1:B:213:ARG:N | 2.35 | 0.58 |
| 1:B:300:LYS:CG | 1:B:300:LYS:O | 2.51 | 0.58 |
| 1:B:471:SER:HA | 1:B:474:THR:HG23 | 1.84 | 0.58 |
| 1:B:213:ARG:HH11 | 1:B:222:VAL:HB | 1.68 | 0.58 |
| 1:C:430:ILE:HD13 | 1:C:443:LEU:HB3 | 1.84 | 0.58 |
| 1:C:564:ALA:O | 1:C:568:ARG:HG2 | 2.03 | 0.58 |
| 1:A:568:ARG:HE | 1:C:548:VAL:CG1 | 2.16 | 0.58 |
| 1:B:334:PRO:HG2 | 1:C:351:THR:HG21 | 1.85 | 0.58 |
| 1:C:148:ALA:HB2 | 1:C:384:PHE:HE2 | 1.69 | 0.58 |
| 1:A:330:LEU:HG | 1:B:101:TRP:CD2 | 2.38 | 0.58 |
| 1:A:458:MET:O | 1:A:461:LEU:HG | 2.02 | 0.58 |
| 1:B:161:GLU:CD | 1:B:189:TRP:HZ3 | 2.07 | 0.58 |
| 1:C:304:TYR:HE1 | 1:C:305:LEU:CG | 2.15 | 0.58 |
| 1:C:370:TYR:C | 1:C:371:TRP:HE3 | 2.07 | 0.58 |
| 1:B:316:LEU:O | 1:B:320:VAL:HG13 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:302:ILE:HG12 | 1:A:303:GLN:N | 2.16 | 0.58 |
| 1:A:378:SER:HA | 1:A:381:VAL:HG22 | 1.86 | 0.58 |
| 1:B:152:ILE:HB | 1:B:464:PHE:CE1 | 2.35 | 0.58 |
| 1:C:141:TRP:HA | 1:C:144:MET:HE3 | 1.85 | 0.58 |
| 1:C:465:PHE:C | 1:C:465:PHE:CD2 | 2.76 | 0.58 |
| 1:C:389:SER:OG | 1:C:397:PHE:HD1 | 1.87 | 0.57 |
| 1:C:138:THR:HA | 1:C:392:ARG:HH22 | 1.68 | 0.57 |
| 1:C:76:TRP:CZ2 | 1:C:84:PHE:O | 2.56 | 0.57 |
| 1:A:222:VAL:HG23 | 1:A:227:GLU:HG2 | 1.86 | 0.57 |
| 1:A:258:ALA:HB1 | 1:A:280:VAL:HG23 | 1.86 | 0.57 |
| 1:B:283:VAL:HA | 1:B:286:LEU:CG | 2.34 | 0.57 |
| 1:C:114:ILE:HD11 | 1:C:398:ILE:CG1 | 2.35 | 0.57 |
| 1:B:320:VAL:HG23 | 1:B:415:ILE:HG21 | 1.75 | 0.57 |
| 1:B:95:VAL:CG2 | 1:B:527:THR:HG21 | 2.34 | 0.57 |
| 1:C:188:HIS:ND1 | 1:C:370:TYR:CE2 | 2.72 | 0.57 |
| 1:A:402:LEU:O | 1:A:404:VAL:N | 2.37 | 0.57 |
| 1:A:526:ALA:C | 1:A:528:PRO:HD2 | 2.23 | 0.57 |
| 1:C:164:THR:HA | 1:C:431:TRP:HH2 | 1.69 | 0.57 |
| 1:C:298:VAL:HG23 | 1:C:302:ILE:CD1 | 2.30 | 0.57 |
| 1:A:305:LEU:HD12 | 1:A:306:SER:N | 2.19 | 0.57 |
| 1:A:477:GLY:O | 1:A:481:GLN:NE2 | 2.32 | 0.57 |
| 1:B:191:LEU:N | 1:B:191:LEU:HD12 | 2.20 | 0.57 |
| 1:B:384:PHE:CE2 | 1:B:471:SER:HB2 | 2.39 | 0.57 |
| 1:B:369:PHE:HD1 | 1:B:523:ILE:HD11 | 1.59 | 0.57 |
| 1:C:112:PHE:O | 1:C:116:VAL:HG13 | 2.05 | 0.57 |
| 1:C:267:ALA:HB1 | 1:C:451:GLN:HE22 | 1.69 | 0.57 |
| 1:A:568:ARG:HE | 1:C:548:VAL:HG13 | 1.68 | 0.57 |
| 1:B:544:LEU:O | 1:B:547:ASP:HB2 | 2.05 | 0.57 |
| 1:C:224:LEU:CD1 | 1:C:539:ALA:CB | 2.83 | 0.57 |
| 1:A:424:GLU:N | 1:A:424:GLU:OE1 | 2.38 | 0.57 |
| 1:A:449:GLY:HA2 | 1:A:452:ILE:HG23 | 1.86 | 0.57 |
| 1:B:161:GLU:CD | 1:B:189:TRP:CZ3 | 2.78 | 0.57 |
| 1:B:399:LEU:HB2 | 1:B:403:LEU:HD13 | 1.87 | 0.57 |
| 1:C:144:MET:SD | 1:C:388:ILE:CG1 | 2.93 | 0.57 |
| 1:A:449:GLY:CA | 1:A:452:ILE:HG23 | 2.34 | 0.57 |
| 1:B:108:THR:OG1 | 1:B:192:HIS:HE1 | 1.87 | 0.57 |
| 1:C:303:GLN:OE1 | 1:C:306:SER:HB3 | 2.05 | 0.57 |
| 1:C:114:ILE:HD11 | 1:C:398:ILE:HG12 | 1.85 | 0.57 |
| 1:C:76:TRP:NE1 | 1:C:85:THR:HB | 2.17 | 0.57 |
| 1:A:235:GLY:N | 1:A:238:ILE:HD13 | 2.20 | 0.56 |
| 1:A:519:GLN:O | 1:A:519:GLN:HG3 | 2.04 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:327:VAL:CG2 | 1:B:328:SER:N | 2.53 | 0.56 |
| 1:C:304:TYR:HD1 | 1:C:305:LEU:H | 1.33 | 0.56 |
| 1:C:144:MET:SD | 1:C:388:ILE:HD13 | 2.45 | 0.56 |
| 1:B:103:PHE:CD1 | 1:B:371:TRP:CB | 2.85 | 0.56 |
| 1:C:380:PHE:CZ | 2:C:2486:CHT:H82 | 2.40 | 0.56 |
| 1:C:69:ILE:N | 1:C:69:ILE:HD12 | 2.20 | 0.56 |
| 1:A:527:THR:CG2 | 1:A:528:PRO:CD | 2.83 | 0.56 |
| 1:A:330:LEU:HD21 | 1:B:101:TRP:CE2 | 2.40 | 0.56 |
| 1:B:156:PHE:O | 1:B:160:THR:HG22 | 2.05 | 0.56 |
| 1:C:475:VAL:HG12 | 1:C:479:MET:HE2 | 1.87 | 0.56 |
| 1:A:574:ARG:HD3 | 1:A:574:ARG:N | 2.17 | 0.56 |
| 1:B:217:LEU:H | 1:B:217:LEU:HD12 | 1.68 | 0.56 |
| 1:C:465:PHE:HD2 | 1:C:465:PHE:C | 2.09 | 0.56 |
| 1:A:204:ILE:HD11 | 1:A:217:LEU:HD12 | 1.86 | 0.56 |
| 1:A:460:LEU:HD11 | 1:A:464:PHE:CZ | 2.40 | 0.56 |
| 1:B:141:TRP:HA | 1:B:144:MET:CE | 2.36 | 0.56 |
| 1:B:352:ALA:HB2 | 1:B:363:LEU:HD12 | 1.87 | 0.56 |
| 1:B:320:VAL:HG21 | 1:B:415:ILE:HG22 | 1.86 | 0.56 |
| 1:B:544:LEU:C | 1:B:546:ASN:H | 2.07 | 0.56 |
| 1:C:394:ILE:HG22 | 1:C:398:ILE:HD12 | 1.87 | 0.56 |
| 1:A:106:PHE:CD1 | 1:A:534:ILE:HD12 | 2.40 | 0.56 |
| 1:A:309:ASN:O | 1:A:313:ALA:CB | 2.54 | 0.56 |
| 1:C:530:LEU:O | 1:C:534:ILE:HG13 | 2.06 | 0.56 |
| 1:C:197:TYR:HE1 | 1:C:374:TRP:O | 1.88 | 0.56 |
| 1:C:250:THR:CG2 | 1:C:377:TRP:HE1 | 2.13 | 0.56 |
| 1:C:92:LEU:HD13 | 1:C:520:ASN:CB | 2.36 | 0.56 |
| 1:C:260:GLN:CD | 1:C:461:LEU:CD2 | 2.71 | 0.56 |
| 1:A:215:GLN:HB2 | 1:A:483:GLY:O | 2.04 | 0.56 |
| 1:B:161:GLU:HG3 | 1:B:165:PHE:CE2 | 2.40 | 0.56 |
| 1:B:288:LEU:O | 1:B:291:ILE:HG22 | 2.06 | 0.56 |
| 1:A:161:GLU:HA | 1:A:164:THR:HG22 | 1.88 | 0.56 |
| 1:A:227:GLU:O | 1:A:228:LYS:HB2 | 2.06 | 0.56 |
| 1:A:261:ILE:CD1 | 1:A:461:LEU:HD21 | 2.34 | 0.56 |
| 1:B:309:ASN:HD21 | 1:B:464:PHE:HD2 | 0.67 | 0.56 |
| 1:C:163:LEU:HD21 | 1:C:431:TRP:HE3 | 1.71 | 0.56 |
| 1:A:159:THR:HG21 | 1:A:440:LEU:HA | 1.88 | 0.56 |
| 1:C:152:ILE:HD13 | 1:C:461:LEU:HG | 1.87 | 0.56 |
| 1:A:206:TYR:CE2 | 1:A:543:ASP:OD2 | 2.59 | 0.55 |
| 1:A:548:VAL:HG23 | 1:A:549:ILE:N | 2.20 | 0.55 |
| 1:C:321:PHE:CE1 | 1:C:326:THR:HG23 | 2.41 | 0.55 |
| 1:C:430:ILE:CD1 | 1:C:443:LEU:HB3 | 2.36 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:344:PHE:O | 1:A:344:PHE:HD2 | 1.86 | 0.55 |
| 1:A:94:ALA:O | 1:A:98:ASN:ND2 | 2.37 | 0.55 |
| 1:B:309:ASN:ND2 | 1:B:464:PHE:HB3 | 2.20 | 0.55 |
| 1:B:95:VAL:CG2 | 1:B:527:THR:CG2 | 2.84 | 0.55 |
| 1:C:92:LEU:O | 1:C:95:VAL:HG12 | 2.06 | 0.55 |
| 1:A:246:THR:HG21 | 1:A:476:MET:HB3 | 1.89 | 0.55 |
| 1:B:251:ALA:HA | 1:B:254:LEU:HG | 1.88 | 0.55 |
| 1:B:103:PHE:HB3 | 1:B:371:TRP:HD1 | 1.72 | 0.55 |
| 1:A:106:PHE:CB | 1:A:534:ILE:HD11 | 2.35 | 0.55 |
| 1:A:408:VAL:HG23 | 1:A:409:SER:N | 2.21 | 0.55 |
| 1:A:121:LYS:HD2 | 1:A:553:TYR:CZ | 2.41 | 0.55 |
| 1:A:92:LEU:HD13 | 1:A:96:VAL:CG2 | 2.35 | 0.55 |
| 1:B:202:LEU:HD23 | 1:B:540:LEU:CD2 | 2.35 | 0.55 |
| 1:B:373:TRP:CD1 | 1:B:374:TRP:N | 2.74 | 0.55 |
| 1:C:304:TYR:C | 1:C:304:TYR:CD1 | 2.80 | 0.55 |
| 1:C:224:LEU:CD1 | 1:C:539:ALA:HA | 2.34 | 0.55 |
| 1:C:291:ILE:HD12 | 1:C:469:ALA:CB | 2.36 | 0.55 |
| 1:A:265:LEU:HA | 1:A:458:MET:HE1 | 1.89 | 0.55 |
| 1:B:305:LEU:HB3 | 1:B:467:THR:HG22 | 1.89 | 0.55 |
| 1:B:167:ARG:NH1 | 1:B:424:GLU:OE2 | 2.40 | 0.55 |
| 1:B:92:LEU:HD21 | 1:B:523:ILE:HG13 | 1.87 | 0.55 |
| 1:C:156:PHE:CD1 | 1:C:256:LEU:HD13 | 2.41 | 0.55 |
| 1:A:114:ILE:HG13 | 1:A:115:VAL:N | 2.22 | 0.55 |
| 1:A:60:TRP:CA | 1:A:63:ILE:HG22 | 2.19 | 0.55 |
| 1:A:70:VAL:O | 1:A:74:VAL:HG23 | 2.07 | 0.55 |
| 1:C:270:ILE:HA | 1:C:271:ILE:CG1 | 2.36 | 0.55 |
| 1:A:113:PHE:HE1 | 1:A:117:ILE:HD11 | 1.67 | 0.55 |
| 1:C:292:PHE:O | 1:C:296:SER:CB | 2.53 | 0.55 |
| 1:C:435:ALA:O | 1:C:439:GLN:OE1 | 2.24 | 0.55 |
| 1:C:477:GLY:O | 1:C:481:GLN:HG3 | 2.07 | 0.55 |
| 1:A:112:PHE:O | 1:A:116:VAL:HG12 | 2.06 | 0.55 |
| 1:C:63:ILE:HG12 | 1:C:480:SER:HB2 | 1.88 | 0.55 |
| 1:A:463:THR:O | 1:A:467:THR:HG23 | 2.07 | 0.54 |
| 1:A:574:ARG:H | 1:A:574:ARG:HD3 | 1.72 | 0.54 |
| 1:B:286:LEU:HD12 | 1:B:287:THR:HG23 | 1.88 | 0.54 |
| 1:C:114:ILE:HG13 | 1:C:398:ILE:HG12 | 1.89 | 0.54 |
| 1:C:398:ILE:HG22 | 1:C:399:LEU:N | 2.21 | 0.54 |
| 1:C:491:VAL:O | 1:C:494:ALA:HB3 | 2.07 | 0.54 |
| 1:B:167:ARG:NH1 | 1:B:424:GLU:OE1 | 2.36 | 0.54 |
| 1:B:186:MET:CG | 1:B:190:THR:HG21 | 2.32 | 0.54 |
| 1:B:463:THR:O | 1:B:465:PHE:N | 2.33 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:72:ALA:O | 1:C:76:TRP:HB3 | 2.07 | 0.54 |
| 1:A:149:GLY:HA2 | 1:A:194:TRP:CH2 | 2.41 | 0.54 |
| 1:A:183:SER:C | 1:A:347:MET:HE1 | 2.27 | 0.54 |
| 1:B:426:ASN:HB3 | 1:B:428:GLU:OE1 | 2.06 | 0.54 |
| 1:C:375:ILE:CD1 | 1:C:530:LEU:HB2 | 2.36 | 0.54 |
| 1:A:460:LEU:HD12 | 1:A:460:LEU:O | 2.07 | 0.54 |
| 1:C:166:TYR:CE2 | 1:C:176:HIS:HD2 | 2.25 | 0.54 |
| 1:C:230:ALA:O | 1:C:231:GLU:HG2 | 2.06 | 0.54 |
| 1:A:123:GLY:HA2 | 1:A:394:ILE:CG2 | 2.37 | 0.54 |
| 1:A:222:VAL:O | 1:A:226:GLY:C | 2.46 | 0.54 |
| 1:B:162:PRO:HG3 | 1:B:185:THR:HG21 | 1.90 | 0.54 |
| 1:B:359:ALA:O | 1:B:360:GLY:C | 2.46 | 0.54 |
| 1:C:298:VAL:CG2 | 1:C:302:ILE:HD13 | 2.34 | 0.54 |
| 1:B:138:THR:O | 1:B:142:ILE:HG23 | 2.07 | 0.54 |
| 1:B:261:ILE:HG23 | 1:B:458:MET:HE1 | 1.89 | 0.54 |
| 1:B:327:VAL:O | 1:B:330:LEU:N | 2.41 | 0.54 |
| 1:B:103:PHE:HE1 | 1:B:372:ALA:HA | 1.72 | 0.54 |
| 1:B:200:VAL:CG1 | 1:B:382:GLY:HA3 | 2.37 | 0.54 |
| 1:C:190:THR:O | 1:C:193:PRO:CG | 2.56 | 0.54 |
| 1:C:428:GLU:N | 1:C:428:GLU:OE1 | 2.41 | 0.54 |
| 1:A:159:THR:OG1 | 1:A:443:LEU:HD21 | 2.08 | 0.54 |
| 1:B:191:LEU:CD1 | 1:B:191:LEU:N | 2.71 | 0.54 |
| 1:B:305:LEU:HB3 | 1:B:467:THR:HG21 | 1.89 | 0.54 |
| 1:C:65:PRO:HB2 | 1:C:240:ILE:HD11 | 1.90 | 0.54 |
| 1:C:163:LEU:HD21 | 1:C:431:TRP:CE3 | 2.42 | 0.54 |
| 1:C:526:ALA:C | 1:C:528:PRO:HD2 | 2.27 | 0.54 |
| 1:A:73:THR:HA | 1:A:76:TRP:HB3 | 1.88 | 0.54 |
| 1:A:92:LEU:HD22 | 1:A:523:ILE:HD11 | 1.88 | 0.54 |
| 1:C:92:LEU:CD1 | 1:C:520:ASN:HA | 2.32 | 0.54 |
| 1:C:430:ILE:HG21 | 1:C:443:LEU:HA | 1.90 | 0.54 |
| 1:A:351:THR:C | 1:A:353:MET:N | 2.60 | 0.53 |
| 1:A:66:ALA:HB3 | 1:A:67:LEU:HD12 | 1.90 | 0.53 |
| 1:B:366:TRP:O | 1:B:370:TYR:CG | 2.61 | 0.53 |
| 1:B:411:VAL:O | 1:B:414:SER:HB2 | 2.07 | 0.53 |
| 1:A:123:GLY:O | 1:A:394:ILE:HB | 2.08 | 0.53 |
| 1:A:344:PHE:HD2 | 1:A:345:PHE:N | 2.05 | 0.53 |
| 1:B:279:ILE:O | 1:B:282:ILE:HG12 | 2.07 | 0.53 |
| 1:B:401:VAL:HG13 | 1:B:402:LEU:HD12 | 1.90 | 0.53 |
| 1:C:82:ASP:O | 1:C:85:THR:HG22 | 2.07 | 0.53 |
| 1:C:81:LYS:HD3 | 1:C:84:PHE:CE2 | 2.44 | 0.53 |
| 1:A:206:TYR:CD2 | 1:A:544:LEU:CD1 | 2.92 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:156:PHE:HB3 | 1:B:260:GLN:OE1 | 2.09 | 0.53 |
| 1:C:106:PHE:CD1 | 1:C:534:ILE:HD13 | 2.43 | 0.53 |
| 1:A:538:PHE:HA | 1:A:541:VAL:HG12 | 1.91 | 0.53 |
| 1:C:112:PHE:O | 1:C:113:PHE:C | 2.47 | 0.53 |
| 1:C:363:LEU:HD23 | 1:C:367:THR:CG2 | 2.30 | 0.53 |
| 1:C:264:GLY:O | 1:C:458:MET:HE1 | 2.09 | 0.53 |
| 1:A:101:TRP:CD2 | 1:A:102:ALA:N | 2.76 | 0.53 |
| 1:A:377:TRP:O | 1:A:381:VAL:HG22 | 2.08 | 0.53 |
| 1:B:103:PHE:CD1 | 1:B:371:TRP:HB2 | 2.43 | 0.53 |
| 1:C:208:THR:HG21 | 1:C:215:GLN:CG | 2.37 | 0.53 |
| 1:A:105:LEU:O | 1:A:109:VAL:HG23 | 2.09 | 0.53 |
| 1:A:345:PHE:CZ | 1:C:341:LEU:HD13 | 2.44 | 0.53 |
| 1:A:412:TRP:CE2 | 1:A:416:PHE:CD2 | 2.97 | 0.53 |
| 1:B:103:PHE:HD1 | 1:B:371:TRP:HB2 | 1.71 | 0.53 |
| 1:B:186:MET:CG | 1:B:190:THR:CG2 | 2.87 | 0.53 |
| 1:B:395:ARG:O | 1:B:399:LEU:HG | 2.07 | 0.53 |
| 1:B:103:PHE:H | 1:B:103:PHE:HD2 | 1.57 | 0.53 |
| 1:A:95:VAL:O | 1:A:99:LEU:HB2 | 2.08 | 0.53 |
| 1:B:545:SER:O | 1:B:550:TYR:HD2 | 1.91 | 0.53 |
| 1:C:339:ASN:O | 1:C:343:ASN:N | 2.35 | 0.53 |
| 1:A:178:VAL:O | 1:A:182:MET:HG2 | 2.08 | 0.53 |
| 1:B:83:SER:O | 1:B:86:ASN:HB2 | 2.09 | 0.53 |
| 1:C:314:ALA:O | 1:C:318:ILE:HG13 | 2.09 | 0.53 |
| 1:C:323:VAL:HG13 | 1:C:324:GLY:H | 1.74 | 0.53 |
| 1:A:369:PHE:HE1 | 1:A:519:GLN:CB | 2.11 | 0.52 |
| 1:A:370:TYR:HB3 | 1:A:374:TRP:HE1 | 1.74 | 0.52 |
| 1:C:188:HIS:HB3 | 1:C:370:TYR:CG | 2.44 | 0.52 |
| 1:C:527:THR:N | 1:C:528:PRO:CD | 2.72 | 0.52 |
| 1:A:202:LEU:HD21 | 1:A:394:ILE:HD13 | 1.90 | 0.52 |
| 1:B:201:GLY:HA2 | 1:B:382:GLY:O | 2.09 | 0.52 |
| 1:B:208:THR:HG21 | 1:B:215:GLN:CA | 2.39 | 0.52 |
| 1:B:464:PHE:CA | 1:B:467:THR:HG23 | 2.36 | 0.52 |
| 1:C:156:PHE:CG | 1:C:256:LEU:HD13 | 2.44 | 0.52 |
| 1:C:134:PRO:CG | 1:C:392:ARG:HD3 | 2.38 | 0.52 |
| 1:A:165:PHE:CE1 | 1:A:362:TRP:HZ2 | 2.28 | 0.52 |
| 1:A:188:HIS:HA | 1:A:371:TRP:CH2 | 2.44 | 0.52 |
| 1:A:222:VAL:N | 1:A:223:PRO:CD | 2.72 | 0.52 |
| 1:A:222:VAL:O | 1:A:226:GLY:O | 2.27 | 0.52 |
| 1:A:437:GLU:O | 1:A:441:PHE:CE1 | 2.63 | 0.52 |
| 1:B:299:GLY:O | 1:B:300:LYS:HB3 | 2.08 | 0.52 |
| 1:C:286:LEU:O | 1:C:290:PHE:HD2 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:291:ILE:HG13 | 1:C:470:ASP:OD1 | 2.10 | 0.52 |
| 1:A:332:LEU:HD23 | 1:A:332:LEU:O | 2.09 | 0.52 |
| 1:C:209:PHE:CE2 | 1:C:390:ARG:HB2 | 2.43 | 0.52 |
| 1:A:248:PHE:CD2 | 1:A:248:PHE:N | 2.77 | 0.52 |
| 1:B:186:MET:HE2 | 1:B:336:SER:HB3 | 1.91 | 0.52 |
| 1:A:330:LEU:HD21 | 1:B:101:TRP:CZ2 | 2.45 | 0.52 |
| 1:B:426:ASN:CB | 1:B:428:GLU:OE1 | 2.57 | 0.52 |
| 1:B:375:ILE:CG2 | 1:B:526:ALA:HB1 | 2.38 | 0.52 |
| 1:C:553:TYR:CD2 | 1:C:554:ARG:N | 2.77 | 0.52 |
| 1:C:77:GLY:O | 1:C:82:ASP:HA | 2.09 | 0.52 |
| 1:A:351:THR:CG2 | 1:C:331:ASN:CB | 2.75 | 0.52 |
| 1:A:81:LYS:HB2 | 1:A:84:PHE:CB | 2.31 | 0.52 |
| 1:B:307:ASN:HA | 1:B:310:MET:HE2 | 1.90 | 0.52 |
| 1:C:231:GLU:HA | 1:C:235:GLY:HA3 | 1.92 | 0.52 |
| 1:C:451:GLN:O | 1:C:455:ILE:HG13 | 2.10 | 0.52 |
| 1:C:475:VAL:HG12 | 1:C:479:MET:CE | 2.40 | 0.52 |
| 1:A:572:GLU:HA | 1:A:575:LYS:HG2 | 1.92 | 0.52 |
| 1:B:116:VAL:O | 1:B:116:VAL:HG12 | 2.09 | 0.52 |
| 1:C:231:GLU:HA | 1:C:234:LEU:O | 2.10 | 0.52 |
| 1:A:80:PHE:CG | 1:A:81:LYS:N | 2.78 | 0.52 |
| 1:B:123:GLY:HA2 | 1:B:394:ILE:CG1 | 2.40 | 0.52 |
| 1:B:127:LEU:HD11 | 1:B:205:ALA:CB | 2.38 | 0.52 |
| 1:B:145:MET:HG3 | 1:B:404:VAL:HG11 | 1.91 | 0.52 |
| 1:A:176:HIS:HB3 | 1:B:356:ASP:OD1 | 2.09 | 0.52 |
| 1:C:70:VAL:CG1 | 1:C:71:LEU:N | 2.73 | 0.52 |
| 1:A:188:HIS:HA | 1:A:371:TRP:HH2 | 1.76 | 0.51 |
| 1:A:485:LEU:O | 1:A:486:GLU:C | 2.48 | 0.51 |
| 1:B:157:TYR:HA | 1:B:160:THR:CG2 | 2.40 | 0.51 |
| 1:C:114:ILE:CD1 | 1:C:398:ILE:HG12 | 2.40 | 0.51 |
| 1:A:154:LEU:O | 1:A:158:GLY:CA | 2.57 | 0.51 |
| 1:A:334:PRO:HG3 | 1:B:104:ILE:CD1 | 2.39 | 0.51 |
| 1:C:184:THR:HG22 | 1:C:188:HIS:CE1 | 2.44 | 0.51 |
| 1:C:320:VAL:HA | 1:C:323:VAL:CG1 | 2.41 | 0.51 |
| 1:B:530:LEU:C | 1:B:530:LEU:HD23 | 2.30 | 0.51 |
| 1:C:153:ASP:OD2 | 2:C:2486:CHT:O6 | 2.26 | 0.51 |
| 1:A:392:ARG:HD2 | 1:A:396:GLU:CG | 2.40 | 0.51 |
| 1:B:291:ILE:HA | 1:B:466:ILE:HD11 | 1.92 | 0.51 |
| 1:A:423:PHE:HB3 | 1:A:428:GLU:O | 2.10 | 0.51 |
| 1:A:309:ASN:ND2 | 1:A:464:PHE:CE1 | 2.76 | 0.51 |
| 1:A:110:PHE:CE1 | 1:A:534:ILE:HD13 | 2.46 | 0.51 |
| 1:B:230:ALA:O | 1:B:232:GLY:N | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:231:GLU:HG3 | 1:B:236:LYS:CE | 2.40 | 0.51 |
| 1:B:463:THR:C | 1:B:465:PHE:H | 2.14 | 0.51 |
| 1:C:183:SER:HB3 | 1:C:339:ASN:HB3 | 1.92 | 0.51 |
| 1:A:160:THR:HG22 | 1:A:439:GLN:HB2 | 1.92 | 0.51 |
| 1:A:80:PHE:CE2 | 1:A:81:LYS:HG2 | 2.45 | 0.51 |
| 1:B:329:ILE:HD11 | 1:B:415:ILE:HG23 | 1.91 | 0.51 |
| 1:B:352:ALA:C | 1:B:354:SER:H | 2.14 | 0.51 |
| 1:C:121:LYS:CD | 1:C:121:LYS:N | 2.56 | 0.51 |
| 1:C:253:SER:OG | 1:C:377:TRP:HH2 | 1.92 | 0.51 |
| 1:C:320:VAL:HA | 1:C:323:VAL:HG12 | 1.93 | 0.51 |
| 1:A:282:ILE:O | 1:A:285:VAL:HG22 | 2.10 | 0.51 |
| 1:B:265:LEU:HB3 | 1:B:269:ASN:HD21 | 1.76 | 0.51 |
| 1:B:320:VAL:HG21 | 1:B:415:ILE:CG2 | 2.39 | 0.51 |
| 1:B:352:ALA:C | 1:B:354:SER:N | 2.64 | 0.51 |
| 1:B:372:ALA:O | 1:B:375:ILE:HG22 | 2.11 | 0.51 |
| 1:A:206:TYR:CD2 | 1:A:544:LEU:HD12 | 2.46 | 0.51 |
| 1:A:351:THR:HG21 | 1:C:331:ASN:CB | 2.30 | 0.51 |
| 1:B:431:TRP:O | 1:B:432:GLY:O | 2.28 | 0.51 |
| 1:C:523:ILE:O | 1:C:527:THR:HG23 | 2.10 | 0.51 |
| 1:A:351:THR:O | 1:A:354:SER:N | 2.32 | 0.51 |
| 1:A:379:PRO:O | 1:A:383:MET:HG2 | 2.10 | 0.51 |
| 1:B:136:PHE:CE2 | 1:B:144:MET:SD | 3.04 | 0.51 |
| 1:B:153:ASP:HA | 1:B:156:PHE:CE2 | 2.46 | 0.51 |
| 1:B:206:TYR:HE2 | 1:B:543:ASP:OD2 | 1.91 | 0.51 |
| 1:C:364:GLY:HA2 | 1:C:368:ILE:HG21 | 1.93 | 0.51 |
| 1:A:350:ARG:CD | 1:A:363:LEU:HD21 | 2.40 | 0.51 |
| 1:A:164:THR:HG21 | 1:A:366:TRP:CH2 | 2.46 | 0.51 |
| 1:A:430:ILE:HG21 | 1:A:443:LEU:HB3 | 1.92 | 0.51 |
| 1:A:443:LEU:C | 1:A:443:LEU:HD12 | 2.31 | 0.51 |
| 1:A:197:TYR:CD1 | 1:A:381:VAL:HG21 | 2.46 | 0.50 |
| 1:A:252:CYS:HB2 | 1:A:522:THR:HG21 | 1.93 | 0.50 |
| 1:A:415:ILE:O | 1:A:419:THR:HG23 | 2.11 | 0.50 |
| 1:B:153:ASP:CG | 1:B:154:LEU:HD23 | 2.31 | 0.50 |
| 1:B:208:THR:OG1 | 1:B:209:PHE:HD1 | 1.94 | 0.50 |
| 1:B:92:LEU:HD12 | 1:B:524:VAL:CG1 | 2.40 | 0.50 |
| 1:C:252:CYS:HA | 1:C:518:LEU:HD11 | 1.92 | 0.50 |
| 1:B:177:ASN:O | 1:B:177:ASN:OD1 | 2.29 | 0.50 |
| 1:B:206:TYR:CE1 | 1:B:210:ARG:HG2 | 2.46 | 0.50 |
| 1:A:222:VAL:CB | 1:A:227:GLU:HG2 | 2.41 | 0.50 |
| 1:A:293:SER:O | 1:A:298:VAL:N | 2.42 | 0.50 |
| 1:C:161:GLU:HG3 | 1:C:185:THR:CG2 | 2.41 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:167:ARG:NH1 | 1:C:431:TRP:CG | 2.78 | 0.50 |
| 1:A:334:PRO:HB3 | 1:B:105:LEU:HD13 | 1.93 | 0.50 |
| 1:A:206:TYR:HE2 | 1:A:543:ASP:OD1 | 1.93 | 0.50 |
| 1:B:136:PHE:CZ | 1:B:144:MET:SD | 3.05 | 0.50 |
| 1:B:216:LEU:HD23 | 1:B:218:SER:H | 1.77 | 0.50 |
| 1:B:126:ARG:HA | 1:B:393:SER:HA | 1.92 | 0.50 |
| 1:B:404:VAL:N | 1:B:405:PRO:CD | 2.74 | 0.50 |
| 1:A:351:THR:HG21 | 1:C:331:ASN:O | 2.12 | 0.50 |
| 1:A:381:VAL:O | 1:A:385:LEU:HD12 | 2.11 | 0.50 |
| 1:B:283:VAL:HG13 | 1:B:286:LEU:HD11 | 1.93 | 0.50 |
| 1:C:165:PHE:CE1 | 1:C:362:TRP:CZ2 | 2.99 | 0.50 |
| 1:A:260:GLN:HA | 1:A:437:GLU:CG | 2.35 | 0.50 |
| 1:C:159:THR:HG21 | 1:C:443:LEU:CD2 | 2.41 | 0.50 |
| 1:B:341:LEU:HD23 | 1:C:345:PHE:CZ | 2.47 | 0.50 |
| 1:C:141:TRP:HD1 | 1:C:388:ILE:CG2 | 2.25 | 0.50 |
| 1:A:321:PHE:CZ | 1:A:326:THR:CG2 | 2.95 | 0.50 |
| 1:B:106:PHE:HB3 | 1:B:110:PHE:CZ | 2.47 | 0.50 |
| 1:B:141:TRP:HA | 1:B:144:MET:HE2 | 1.94 | 0.50 |
| 1:B:329:ILE:CG2 | 1:B:415:ILE:HG13 | 2.41 | 0.50 |
| 1:C:116:VAL:HA | 1:C:119:ALA:HB3 | 1.94 | 0.50 |
| 1:A:206:TYR:HE2 | 1:A:543:ASP:OD2 | 1.93 | 0.50 |
| 1:A:380:PHE:CD1 | 1:A:472:ALA:HA | 2.46 | 0.50 |
| 1:A:92:LEU:HD23 | 1:A:520:ASN:CG | 2.32 | 0.50 |
| 1:B:67:LEU:O | 1:B:70:VAL:HG12 | 2.11 | 0.50 |
| 1:C:163:LEU:CD2 | 1:C:431:TRP:CZ3 | 2.95 | 0.50 |
| 1:C:186:MET:HE3 | 1:C:190:THR:CG2 | 2.40 | 0.50 |
| 1:C:282:ILE:O | 1:C:286:LEU:HD23 | 2.12 | 0.50 |
| 1:C:92:LEU:HA | 1:C:95:VAL:HG12 | 1.93 | 0.50 |
| 1:A:137:ARG:HD3 | 1:A:138:THR:H | 1.76 | 0.50 |
| 1:A:207:SER:O | 1:A:213:ARG:HG2 | 2.12 | 0.50 |
| 1:A:548:VAL:HG23 | 1:A:549:ILE:H | 1.75 | 0.50 |
| 1:B:366:TRP:C | 1:B:370:TYR:HD2 | 2.14 | 0.50 |
| 1:B:538:PHE:HA | 1:B:541:VAL:HG12 | 1.94 | 0.50 |
| 1:C:218:SER:C | 1:C:220:ALA:H | 2.15 | 0.50 |
| 1:B:318:ILE:O | 1:B:322:VAL:HG22 | 2.12 | 0.49 |
| 1:A:276:ASP:N | 1:A:279:ILE:HG13 | 2.27 | 0.49 |
| 1:B:103:PHE:N | 1:B:103:PHE:CD2 | 2.79 | 0.49 |
| 1:B:379:PRO:O | 1:B:383:MET:SD | 2.71 | 0.49 |
| 1:B:323:VAL:HG23 | 1:B:324:GLY:N | 2.26 | 0.49 |
| 1:B:210:ARG:NH2 | 1:B:547:ASP:OD1 | 2.45 | 0.49 |
| 1:A:412:TRP:O | 1:A:416:PHE:HD2 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:574:ARG:H | 1:A:574:ARG:CD | 2.22 | 0.49 |
| 1:A:577:GLU:HG3 | 1:A:578:LEU:N | 2.27 | 0.49 |
| 1:B:213:ARG:HH12 | 1:B:223:PRO:HD3 | 1.78 | 0.49 |
| 1:B:544:LEU:O | 1:B:547:ASP:N | 2.39 | 0.49 |
| 1:C:173:HIS:CD2 | 1:C:180:VAL:CB | 2.95 | 0.49 |
| 1:C:181:ALA:O | 1:C:185:THR:HG23 | 2.12 | 0.49 |
| 1:C:337:ILE:CD1 | 1:C:410:THR:HG21 | 2.36 | 0.49 |
| 1:C:103:PHE:CZ | 1:C:530:LEU:HD22 | 2.47 | 0.49 |
| 1:A:206:TYR:CE1 | 1:A:210:ARG:HG2 | 2.47 | 0.49 |
| 1:A:378:SER:N | 1:A:379:PRO:CD | 2.76 | 0.49 |
| 1:A:194:TRP:CE3 | 1:A:401:VAL:HG13 | 2.47 | 0.49 |
| 1:B:117:ILE:HG23 | 1:B:398:ILE:HD13 | 1.94 | 0.49 |
| 1:B:193:PRO:HB3 | 1:B:374:TRP:CD2 | 2.48 | 0.49 |
| 1:B:352:ALA:O | 1:B:354:SER:N | 2.46 | 0.49 |
| 1:A:466:ILE:HD12 | 1:A:467:THR:N | 2.28 | 0.49 |
| 1:B:77:GLY:O | 1:B:82:ASP:OD1 | 2.30 | 0.49 |
| 1:B:112:PHE:O | 1:B:116:VAL:HG23 | 2.13 | 0.49 |
| 1:B:163:LEU:HD11 | 1:B:167:ARG:HD2 | 1.94 | 0.49 |
| 1:B:205:ALA:HB2 | 1:B:386:ALA:CB | 2.37 | 0.49 |
| 1:C:304:TYR:C | 1:C:304:TYR:HD1 | 2.08 | 0.49 |
| 1:C:401:VAL:O | 1:C:405:PRO:CD | 2.58 | 0.49 |
| 1:C:452:ILE:HA | 1:C:455:ILE:HD12 | 1.95 | 0.49 |
| 1:C:67:LEU:HD23 | 1:C:70:VAL:HG11 | 1.94 | 0.49 |
| 1:A:562:ARG:O | 1:A:565:ARG:CB | 2.60 | 0.49 |
| 1:C:67:LEU:HA | 1:C:70:VAL:HG12 | 1.94 | 0.49 |
| 1:A:432:GLY:H | 1:A:439:GLN:HE21 | 1.59 | 0.49 |
| 1:B:103:PHE:CE2 | 1:B:530:LEU:HD12 | 2.47 | 0.49 |
| 1:C:114:ILE:HD12 | 1:C:117:ILE:CD1 | 2.37 | 0.49 |
| 1:C:161:GLU:HB3 | 1:C:162:PRO:CD | 2.43 | 0.49 |
| 1:A:345:PHE:CE1 | 1:C:341:LEU:CD1 | 2.93 | 0.49 |
| 1:A:558:ARG:O | 1:A:562:ARG:HG2 | 2.12 | 0.49 |
| 1:A:563:LEU:C | 1:A:563:LEU:HD23 | 2.33 | 0.49 |
| 1:B:307:ASN:O | 1:B:311:VAL:HG23 | 2.12 | 0.49 |
| 1:C:141:TRP:CD1 | 1:C:388:ILE:CG2 | 2.96 | 0.49 |
| 1:A:215:GLN:NE2 | 1:A:387:ARG:NH2 | 2.61 | 0.48 |
| 1:A:562:ARG:O | 1:A:565:ARG:N | 2.44 | 0.48 |
| 1:B:106:PHE:O | 1:B:107:GLY:C | 2.51 | 0.48 |
| 1:C:251:ALA:O | 1:C:255:GLY:N | 2.37 | 0.48 |
| 1:C:311:VAL:O | 1:C:315:LEU:HD13 | 2.13 | 0.48 |
| 1:C:163:LEU:CD2 | 1:C:431:TRP:CE3 | 2.96 | 0.48 |
| 1:A:114:ILE:HD11 | 1:A:402:LEU:HD11 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:408:VAL:CG2 | 1:A:409:SER:N | 2.76 | 0.48 |
| 1:B:167:ARG:NH1 | 1:B:424:GLU:CD | 2.67 | 0.48 |
| 1:B:541:VAL:HG13 | 1:B:542:LYS:N | 2.28 | 0.48 |
| 1:C:167:ARG:HH21 | 1:C:424:GLU:CD | 2.16 | 0.48 |
| 1:C:64:VAL:N | 1:C:65:PRO:CD | 2.76 | 0.48 |
| 1:B:132:GLU:OE1 | 1:B:390:ARG:CZ | 2.61 | 0.48 |
| 1:C:155:MET:SD | 1:C:461:LEU:HD11 | 2.54 | 0.48 |
| 1:C:459:ILE:O | 1:C:463:THR:HG23 | 2.13 | 0.48 |
| 1:A:219:SER:O | 1:A:222:VAL:HG13 | 2.14 | 0.48 |
| 1:A:60:TRP:CE3 | 1:A:63:ILE:HG21 | 2.48 | 0.48 |
| 1:B:309:ASN:HD22 | 1:B:464:PHE:HB3 | 1.79 | 0.48 |
| 1:B:463:THR:O | 1:B:464:PHE:CD1 | 2.67 | 0.48 |
| 1:B:464:PHE:CD1 | 1:B:465:PHE:N | 2.81 | 0.48 |
| 1:A:565:ARG:HG2 | 1:C:130:ILE:HG21 | 1.95 | 0.48 |
| 1:C:167:ARG:HH22 | 1:C:431:TRP:HB2 | 1.78 | 0.48 |
| 1:C:291:ILE:HD12 | 1:C:469:ALA:HB3 | 1.95 | 0.48 |
| 1:C:466:ILE:HD12 | 1:C:466:ILE:H | 1.79 | 0.48 |
| 1:A:137:ARG:CD | 1:A:139:VAL:HG22 | 2.40 | 0.48 |
| 1:B:453:MET:O | 1:B:456:ILE:CG1 | 2.61 | 0.48 |
| 1:B:58:LEU:O | 1:B:60:TRP:HD1 | 1.96 | 0.48 |
| 1:C:546:ASN:O | 1:C:551:LEU:HD12 | 2.13 | 0.48 |
| 1:A:355:ALA:O | 1:A:356:ASP:CB | 2.61 | 0.48 |
| 1:B:186:MET:HE1 | 1:B:336:SER:CB | 2.43 | 0.48 |
| 1:B:333:LEU:HB2 | 1:B:334:PRO:CD | 2.43 | 0.48 |
| 1:B:372:ALA:CB | 1:B:523:ILE:CG2 | 2.88 | 0.48 |
| 1:B:80:PHE:O | 1:B:80:PHE:CG | 2.67 | 0.48 |
| 1:C:178:VAL:HG23 | 1:C:179:GLY:N | 2.28 | 0.48 |
| 1:C:443:LEU:HG | 1:C:444:LEU:N | 2.29 | 0.48 |
| 1:A:172:GLY:C | 1:A:173:HIS:CG | 2.86 | 0.48 |
| 1:B:118:ALA:HB2 | 1:B:398:ILE:HD12 | 1.96 | 0.48 |
| 1:C:58:LEU:HD12 | 1:C:58:LEU:H | 1.79 | 0.48 |
| 1:C:70:VAL:HG13 | 1:C:71:LEU:N | 2.27 | 0.48 |
| 1:C:74:VAL:HG23 | 1:C:75:VAL:N | 2.29 | 0.48 |
| 1:C:76:TRP:CZ2 | 1:C:84:PHE:C | 2.87 | 0.48 |
| 1:C:132:GLU:OE2 | 1:C:390:ARG:NE | 2.45 | 0.48 |
| 1:C:303:GLN:O | 1:C:304:TYR:CB | 2.59 | 0.48 |
| 1:C:123:GLY:HA3 | 1:C:395:ARG:HB2 | 1.95 | 0.48 |
| 1:C:264:GLY:HA2 | 1:C:441:PHE:CE1 | 2.48 | 0.48 |
| 1:C:497:VAL:HG23 | 1:C:498:ALA:N | 2.29 | 0.48 |
| 1:A:184:THR:N | 1:A:347:MET:HE1 | 2.29 | 0.48 |
| 1:A:371:TRP:CA | 1:A:371:TRP:CE3 | 2.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:321:PHE:HA | 1:B:329:ILE:CD1 | 2.43 | 0.48 |
| 1:B:544:LEU:C | 1:B:546:ASN:N | 2.67 | 0.48 |
| 1:B:114:ILE:HG13 | 1:B:115:VAL:H | 1.78 | 0.48 |
| 1:B:125:ILE:CG2 | 1:B:210:ARG:NH2 | 2.67 | 0.48 |
| 1:C:305:LEU:HA | 1:C:308:ALA:CB | 2.43 | 0.48 |
| 1:C:379:PRO:HD3 | 1:C:529:PHE:HE2 | 1.77 | 0.48 |
| 1:A:106:PHE:HB3 | 1:A:534:ILE:CD1 | 2.44 | 0.47 |
| 1:A:544:LEU:O | 1:A:547:ASP:N | 2.31 | 0.47 |
| 1:B:145:MET:CE | 1:B:404:VAL:HG21 | 2.43 | 0.47 |
| 1:B:77:GLY:O | 1:B:78:ILE:HD13 | 2.14 | 0.47 |
| 1:C:172:GLY:O | 1:C:173:HIS:ND1 | 2.42 | 0.47 |
| 1:C:259:LEU:HD13 | 1:C:437:GLU:OE1 | 2.14 | 0.47 |
| 1:A:121:LYS:HD2 | 1:A:553:TYR:CE2 | 2.49 | 0.47 |
| 1:A:343:ASN:C | 1:A:347:MET:HG3 | 2.29 | 0.47 |
| 1:A:136:PHE:CE2 | 1:A:388:ILE:HG23 | 2.46 | 0.47 |
| 1:A:405:PRO:O | 1:A:408:VAL:HG22 | 2.14 | 0.47 |
| 1:B:192:HIS:CB | 1:B:193:PRO:HD3 | 2.44 | 0.47 |
| 1:B:208:THR:HG21 | 1:B:215:GLN:HB2 | 1.96 | 0.47 |
| 1:B:305:LEU:HA | 1:B:305:LEU:HD12 | 1.72 | 0.47 |
| 1:B:58:LEU:HA | 1:B:481:GLN:HG2 | 1.96 | 0.47 |
| 1:B:379:PRO:HD3 | 1:B:529:PHE:CE2 | 2.48 | 0.47 |
| 1:C:186:MET:CE | 1:C:190:THR:HG21 | 2.42 | 0.47 |
| 1:C:75:VAL:HG12 | 1:C:76:TRP:N | 2.29 | 0.47 |
| 1:A:158:GLY:HA2 | 1:A:413:PHE:CE1 | 2.46 | 0.47 |
| 1:A:473:SER:HA | 1:A:476:MET:CG | 2.43 | 0.47 |
| 1:A:565:ARG:HG2 | 1:C:130:ILE:CG2 | 2.44 | 0.47 |
| 1:A:72:ALA:O | 1:A:76:TRP:CB | 2.61 | 0.47 |
| 1:B:224:LEU:HD11 | 1:B:538:PHE:HB2 | 1.97 | 0.47 |
| 1:B:316:LEU:HD22 | 1:B:460:LEU:HD11 | 1.93 | 0.47 |
| 1:B:259:LEU:CD1 | 1:B:437:GLU:HG2 | 2.43 | 0.47 |
| 1:B:545:SER:O | 1:B:550:TYR:CD2 | 2.67 | 0.47 |
| 1:C:267:ALA:CB | 1:C:451:GLN:HE22 | 2.27 | 0.47 |
| 1:C:378:SER:N | 1:C:379:PRO:HD2 | 2.28 | 0.47 |
| 1:B:145:MET:HE3 | 1:B:404:VAL:CG2 | 2.43 | 0.47 |
| 1:B:371:TRP:HA | 1:B:371:TRP:HE3 | 1.80 | 0.47 |
| 1:B:464:PHE:HA | 1:B:467:THR:OG1 | 2.15 | 0.47 |
| 1:A:423:PHE:HD2 | 1:A:430:ILE:HD11 | 1.80 | 0.47 |
| 1:A:562:ARG:HA | 1:A:565:ARG:HB2 | 1.96 | 0.47 |
| 1:A:574:ARG:HA | 1:A:577:GLU:HG2 | 1.96 | 0.47 |
| 1:C:123:GLY:CA | 1:C:395:ARG:HB2 | 2.44 | 0.47 |
| 1:C:325:PRO:HB2 | 1:C:328:SER:HB2 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:213:ARG:NH1 | 1:A:219:SER:HB3 | 2.29 | 0.47 |
| 1:A:478:THR:CA | 1:A:481:GLN:NE2 | 2.62 | 0.47 |
| 1:C:252:CYS:SG | 1:C:518:LEU:HG | 2.54 | 0.47 |
| 1:A:317:ALA:O | 1:A:320:VAL:HG22 | 2.14 | 0.47 |
| 1:B:132:GLU:OE2 | 1:B:390:ARG:HG3 | 2.15 | 0.47 |
| 1:B:411:VAL:HG13 | 1:B:415:ILE:HD12 | 1.91 | 0.47 |
| 1:A:392:ARG:HD3 | 1:A:392:ARG:HA | 1.52 | 0.47 |
| 1:B:191:LEU:H | 1:B:191:LEU:CD1 | 2.27 | 0.47 |
| 1:B:247:VAL:HG12 | 1:B:248:PHE:HD1 | 1.80 | 0.47 |
| 1:B:378:SER:HB2 | 1:B:379:PRO:HD3 | 1.96 | 0.47 |
| 1:B:430:ILE:C | 1:B:430:ILE:HD12 | 2.35 | 0.47 |
| 1:C:318:ILE:O | 1:C:322:VAL:HG22 | 2.15 | 0.47 |
| 1:C:340:TYR:O | 1:C:344:PHE:N | 2.48 | 0.47 |
| 1:C:209:PHE:CD2 | 1:C:390:ARG:HD2 | 2.50 | 0.47 |
| 1:C:418:GLY:O | 1:C:422:VAL:HG23 | 2.14 | 0.47 |
| 1:A:519:GLN:O | 1:A:520:ASN:HB2 | 2.14 | 0.47 |
| 1:B:135:GLU:OE2 | 1:B:136:PHE:HD2 | 1.98 | 0.47 |
| 1:B:159:THR:HG23 | 1:B:443:LEU:HD23 | 1.97 | 0.47 |
| 1:B:189:TRP:CE3 | 1:B:413:PHE:CZ | 3.03 | 0.47 |
| 1:B:453:MET:O | 1:B:456:ILE:HG12 | 2.15 | 0.47 |
| 1:B:379:PRO:CG | 1:B:529:PHE:CZ | 2.94 | 0.47 |
| 1:C:316:LEU:HB3 | 1:C:416:PHE:HZ | 1.79 | 0.47 |
| 1:A:76:TRP:HZ2 | 1:A:84:PHE:CD2 | 2.32 | 0.47 |
| 1:B:371:TRP:HA | 1:B:371:TRP:CE3 | 2.50 | 0.47 |
| 1:B:309:ASN:CG | 1:B:463:THR:CG2 | 2.82 | 0.47 |
| 1:C:492:THR:HG22 | 1:C:493:ALA:N | 2.30 | 0.47 |
| 1:A:243:ILE:HD12 | 1:A:244:ILE:H | 1.80 | 0.47 |
| 1:A:371:TRP:CE3 | 1:A:371:TRP:N | 2.82 | 0.47 |
| 1:A:148:ALA:HB2 | 1:A:384:PHE:CE2 | 2.50 | 0.47 |
| 1:A:543:ASP:OD1 | 1:A:543:ASP:C | 2.53 | 0.47 |
| 1:B:295:ILE:HD12 | 1:B:295:ILE:N | 2.30 | 0.47 |
| 1:B:322:VAL:HG23 | 1:B:323:VAL:N | 2.29 | 0.47 |
| 1:B:401:VAL:C | 1:B:402:LEU:HD12 | 2.35 | 0.47 |
| 1:B:474:THR:O | 1:B:478:THR:HG23 | 2.14 | 0.47 |
| 1:C:152:ILE:HG21 | 1:C:257:GLY:HA3 | 1.97 | 0.47 |
| 1:C:161:GLU:HB3 | 1:C:162:PRO:HD3 | 1.97 | 0.47 |
| 1:C:269:ASN:C | 1:C:270:ILE:HD12 | 2.35 | 0.47 |
| 1:C:316:LEU:HB3 | 1:C:416:PHE:CZ | 2.50 | 0.47 |
| 1:C:163:LEU:CG | 1:C:431:TRP:CZ3 | 2.89 | 0.47 |
| 1:A:145:MET:SD | 1:A:405:PRO:HD3 | 2.55 | 0.46 |
| 1:B:128:GLY:HA3 | 1:B:390:ARG:HH11 | 1.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:256:LEU:HD12 | 1:C:257:GLY:N | 2.29 | 0.46 |
| 1:A:551:LEU:HD23 | 1:A:551:LEU:HA | 1.75 | 0.46 |
| 1:B:269:ASN:OD1 | 1:B:269:ASN:O | 2.32 | 0.46 |
| 1:C:142:ILE:O | 1:C:145:MET:N | 2.47 | 0.46 |
| 1:C:374:TRP:CE3 | 1:C:374:TRP:HA | 2.50 | 0.46 |
| 1:C:526:ALA:C | 1:C:528:PRO:CD | 2.84 | 0.46 |
| 1:A:353:MET:HG2 | 1:C:332:LEU:HD21 | 1.97 | 0.46 |
| 1:B:146:PHE:CB | 1:B:310:MET:SD | 2.99 | 0.46 |
| 1:C:374:TRP:CE3 | 1:C:374:TRP:CA | 2.99 | 0.46 |
| 1:C:159:THR:HG22 | 1:C:416:PHE:O | 2.16 | 0.46 |
| 1:A:93:SER:O | 1:A:97:ASP:OD1 | 2.34 | 0.46 |
| 1:A:204:ILE:O | 1:A:208:THR:HG23 | 2.15 | 0.46 |
| 1:B:399:LEU:O | 1:B:400:GLY:C | 2.53 | 0.46 |
| 1:B:411:VAL:HA | 1:B:414:SER:HB2 | 1.98 | 0.46 |
| 1:C:559:PHE:HA | 1:C:562:ARG:CG | 2.43 | 0.46 |
| 1:A:302:ILE:HG13 | 1:A:303:GLN:N | 2.18 | 0.46 |
| 1:C:367:THR:HG23 | 1:C:368:ILE:N | 2.30 | 0.46 |
| 1:A:404:VAL:HB | 1:A:405:PRO:CD | 2.45 | 0.46 |
| 1:A:412:TRP:CZ3 | 1:A:416:PHE:HE2 | 2.33 | 0.46 |
| 1:B:105:LEU:HD23 | 1:B:106:PHE:CE2 | 2.51 | 0.46 |
| 1:C:222:VAL:N | 1:C:223:PRO:CD | 2.79 | 0.46 |
| 1:C:81:LYS:O | 1:C:82:ASP:HB3 | 2.15 | 0.46 |
| 1:A:302:ILE:O | 1:A:303:GLN:HB2 | 2.16 | 0.46 |
| 1:A:540:LEU:HD23 | 1:A:540:LEU:C | 2.35 | 0.46 |
| 1:A:64:VAL:O | 1:A:68:VAL:HG12 | 2.16 | 0.46 |
| 1:B:346:GLN:HG3 | 1:B:347:MET:H | 1.80 | 0.46 |
| 1:C:473:SER:CA | 1:C:476:MET:HE2 | 2.45 | 0.46 |
| 1:A:355:ALA:O | 1:A:356:ASP:HB2 | 2.16 | 0.46 |
| 1:B:132:GLU:OE1 | 1:B:390:ARG:NH1 | 2.49 | 0.46 |
| 1:B:95:VAL:HG13 | 1:B:96:VAL:N | 2.31 | 0.46 |
| 1:A:371:TRP:CE3 | 1:A:371:TRP:HA | 2.50 | 0.45 |
| 1:A:407:GLY:HA2 | 1:A:410:THR:HG22 | 1.98 | 0.45 |
| 1:B:238:ILE:HG22 | 1:B:239:ASP:N | 2.30 | 0.45 |
| 1:B:372:ALA:O | 1:B:375:ILE:N | 2.49 | 0.45 |
| 1:B:58:LEU:HG | 1:B:481:GLN:HE21 | 1.81 | 0.45 |
| 1:C:121:LYS:O | 1:C:122:PHE:C | 2.54 | 0.45 |
| 1:C:554:ARG:NH1 | 1:C:557:GLN:NE2 | 2.64 | 0.45 |
| 1:A:302:ILE:HG12 | 1:A:303:GLN:HG3 | 1.98 | 0.45 |
| 1:B:145:MET:SD | 1:B:404:VAL:HG21 | 2.57 | 0.45 |
| 1:C:145:MET:SD | 1:C:404:VAL:HB | 2.56 | 0.45 |
| 1:C:224:LEU:HD11 | 1:C:539:ALA:CB | 2.44 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:141:TRP:CD1 | 1:C:388:ILE:HG22 | 2.51 | 0.45 |
| 1:C:506:LEU:HD21 | 1:C:521:VAL:HG21 | 1.97 | 0.45 |
| 1:B:172:GLY:C | 1:B:173:HIS:CD2 | 2.89 | 0.45 |
| 1:B:231:GLU:O | 1:B:236:LYS:HG2 | 2.16 | 0.45 |
| 1:A:101:TRP:HB3 | 1:C:331:ASN:OD1 | 2.16 | 0.45 |
| 1:A:59:ASN:OD1 | 1:A:482:HIS:NE2 | 2.49 | 0.45 |
| 1:A:252:CYS:HB2 | 1:A:522:THR:CG2 | 2.46 | 0.45 |
| 1:A:67:LEU:HD12 | 1:A:67:LEU:N | 2.32 | 0.45 |
| 1:B:117:ILE:CG2 | 1:B:118:ALA:N | 2.80 | 0.45 |
| 1:B:211:VAL:CG1 | 1:B:213:ARG:HE | 2.23 | 0.45 |
| 1:B:187:PHE:CD1 | 1:B:347:MET:SD | 3.09 | 0.45 |
| 1:C:125:ILE:HD12 | 1:C:544:LEU:HD22 | 1.99 | 0.45 |
| 1:A:163:LEU:HD11 | 1:A:420:ALA:O | 2.17 | 0.45 |
| 1:A:208:THR:O | 1:A:212:GLY:HA2 | 2.16 | 0.45 |
| 1:A:543:ASP:O | 1:A:543:ASP:OD1 | 2.33 | 0.45 |
| 1:C:316:LEU:N | 1:C:316:LEU:CD1 | 2.78 | 0.45 |
| 1:A:542:LYS:HD2 | 1:A:542:LYS:HA | 1.65 | 0.45 |
| 1:B:113:PHE:CZ | 1:B:537:MET:HG3 | 2.52 | 0.45 |
| 1:B:234:LEU:N | 1:B:234:LEU:HD12 | 2.32 | 0.45 |
| 1:B:118:ALA:HB2 | 1:B:398:ILE:HG21 | 1.98 | 0.45 |
| 1:C:213:ARG:HD2 | 1:C:219:SER:O | 2.15 | 0.45 |
| 1:C:167:ARG:NH1 | 1:C:431:TRP:CD2 | 2.84 | 0.45 |
| 1:C:488:ASN:HB3 | 1:C:491:VAL:CG1 | 2.44 | 0.45 |
| 1:C:243:ILE:HG21 | 1:C:495:TRP:CH2 | 2.52 | 0.45 |
| 1:A:113:PHE:HA | 1:A:116:VAL:HG13 | 1.98 | 0.45 |
| 1:A:189:TRP:CH2 | 1:A:370:TYR:OH | 2.70 | 0.45 |
| 1:A:215:GLN:NE2 | 1:A:387:ARG:HH21 | 2.14 | 0.45 |
| 1:A:288:LEU:HD12 | 1:A:289:ALA:N | 2.31 | 0.45 |
| 1:A:376:SER:O | 1:A:377:TRP:HB2 | 2.17 | 0.45 |
| 1:A:387:ARG:NH1 | 1:A:387:ARG:HB3 | 2.29 | 0.45 |
| 1:B:216:LEU:HD21 | 1:B:239:ASP:OD1 | 2.17 | 0.45 |
| 1:B:455:ILE:O | 1:B:458:MET:HB2 | 2.17 | 0.45 |
| 1:C:204:ILE:HD13 | 1:C:383:MET:CG | 2.39 | 0.45 |
| 1:B:331:ASN:O | 1:C:351:THR:HG21 | 2.17 | 0.45 |
| 1:C:537:MET:O | 1:C:541:VAL:HG23 | 2.15 | 0.45 |
| 1:A:204:ILE:HD13 | 1:A:383:MET:SD | 2.56 | 0.45 |
| 1:A:329:ILE:HG23 | 1:A:414:SER:C | 2.36 | 0.45 |
| 1:A:99:LEU:O | 1:A:100:GLY:C | 2.55 | 0.45 |
| 1:A:94:ALA:O | 1:A:98:ASN:HB2 | 2.17 | 0.45 |
| 1:B:355:ALA:O | 1:B:356:ASP:CB | 2.63 | 0.45 |
| 1:C:191:LEU:O | 1:C:195:ALA:N | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:193:PRO:CB | 1:C:374:TRP:CD1 | 2.96 | 0.45 |
| 1:A:330:LEU:HG | 1:B:101:TRP:CG | 2.52 | 0.45 |
| 1:A:402:LEU:O | 1:A:403:LEU:C | 2.56 | 0.45 |
| 1:A:478:THR:CA | 1:A:481:GLN:HE21 | 2.29 | 0.45 |
| 1:A:330:LEU:CD2 | 1:B:101:TRP:CE2 | 2.99 | 0.45 |
| 1:B:358:THR:O | 1:B:360:GLY:N | 2.50 | 0.45 |
| 1:B:373:TRP:HD1 | 1:B:373:TRP:O | 2.00 | 0.45 |
| 1:A:352:ALA:O | 1:A:357:GLY:CA | 2.58 | 0.44 |
| 1:A:110:PHE:CZ | 1:A:534:ILE:HD13 | 2.52 | 0.44 |
| 1:B:103:PHE:HE1 | 1:B:372:ALA:CA | 2.31 | 0.44 |
| 1:B:145:MET:HG2 | 1:B:146:PHE:N | 2.32 | 0.44 |
| 1:B:216:LEU:HD23 | 1:B:218:SER:N | 2.32 | 0.44 |
| 1:B:270:ILE:HA | 1:B:271:ILE:HA | 1.72 | 0.44 |
| 1:B:320:VAL:HG23 | 1:B:321:PHE:N | 2.32 | 0.44 |
| 1:B:326:THR:O | 1:B:330:LEU:HB2 | 2.17 | 0.44 |
| 1:C:211:VAL:O | 1:C:211:VAL:HG12 | 2.17 | 0.44 |
| 1:C:187:PHE:CD1 | 1:C:347:MET:HG3 | 2.52 | 0.44 |
| 1:C:170:VAL:HG11 | 1:C:350:ARG:NH2 | 2.33 | 0.44 |
| 1:C:523:ILE:O | 1:C:527:THR:CG2 | 2.66 | 0.44 |
| 1:A:285:VAL:HA | 1:A:288:LEU:CG | 2.40 | 0.44 |
| 1:A:182:MET:SD | 1:A:332:LEU:HD11 | 2.57 | 0.44 |
| 1:A:578:LEU:O | 1:A:581:LYS:HB3 | 2.17 | 0.44 |
| 1:B:152:ILE:HD11 | 1:B:257:GLY:HA3 | 1.99 | 0.44 |
| 1:B:365:SER:C | 1:B:366:TRP:HD1 | 2.18 | 0.44 |
| 1:B:362:TRP:HZ3 | 1:B:367:THR:HG1 | 1.63 | 0.44 |
| 1:B:188:HIS:NE2 | 1:B:367:THR:OG1 | 2.33 | 0.44 |
| 1:B:468:SER:O | 1:B:472:ALA:HB2 | 2.17 | 0.44 |
| 1:B:534:ILE:O | 1:B:537:MET:HB3 | 2.16 | 0.44 |
| 1:B:70:VAL:HG13 | 1:B:71:LEU:N | 2.31 | 0.44 |
| 1:A:222:VAL:HB | 1:A:227:GLU:CA | 2.37 | 0.44 |
| 1:C:191:LEU:C | 1:C:193:PRO:HD2 | 2.38 | 0.44 |
| 1:C:392:ARG:NH1 | 1:C:396:GLU:OE2 | 2.44 | 0.44 |
| 1:C:452:ILE:HG13 | 1:C:453:MET:N | 2.33 | 0.44 |
| 1:C:152:ILE:CD1 | 1:C:461:LEU:HG | 2.45 | 0.44 |
| 1:A:154:LEU:O | 1:A:158:GLY:N | 2.50 | 0.44 |
| 1:A:402:LEU:O | 1:A:405:PRO:HD2 | 2.16 | 0.44 |
| 1:A:571:ASN:HB3 | 1:A:575:LYS:HE3 | 2.00 | 0.44 |
| 1:B:131:ASP:OD2 | 1:C:565:ARG:CZ | 2.64 | 0.44 |
| 1:B:455:ILE:CG1 | 1:B:456:ILE:N | 2.80 | 0.44 |
| 1:B:378:SER:HB2 | 1:B:529:PHE:HE2 | 1.82 | 0.44 |
| 1:A:559:PHE:C | 1:A:559:PHE:CD2 | 2.91 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:158:GLY:O | 1:B:162:PRO:HD2 | 2.17 | 0.44 |
| 1:B:152:ILE:HD13 | 1:B:253:SER:O | 2.17 | 0.44 |
| 1:B:65:PRO:HB2 | 1:B:240:ILE:HD13 | 2.00 | 0.44 |
| 1:C:154:LEU:O | 1:C:155:MET:C | 2.55 | 0.44 |
| 1:C:374:TRP:HE3 | 1:C:374:TRP:HA | 1.82 | 0.44 |
| 1:C:472:ALA:C | 1:C:476:MET:HE2 | 2.38 | 0.44 |
| 1:A:219:SER:C | 1:A:221:PHE:H | 2.21 | 0.44 |
| 1:A:370:TYR:O | 1:A:374:TRP:CD1 | 2.71 | 0.44 |
| 1:A:155:MET:HB3 | 1:A:440:LEU:HD11 | 2.00 | 0.44 |
| 1:A:88:ALA:HA | 1:A:91:ALA:CB | 2.47 | 0.44 |
| 1:B:159:THR:HG23 | 1:B:443:LEU:CD2 | 2.48 | 0.44 |
| 1:B:354:SER:HA | 1:B:355:ALA:HA | 1.51 | 0.44 |
| 1:B:86:ASN:O | 1:B:89:SER:HB2 | 2.17 | 0.44 |
| 1:C:156:PHE:CD1 | 1:C:256:LEU:HB2 | 2.52 | 0.44 |
| 1:C:319:PHE:CD2 | 1:C:453:MET:HG3 | 2.53 | 0.44 |
| 1:C:493:ALA:O | 1:C:496:GLY:N | 2.51 | 0.44 |
| 1:B:305:LEU:CD2 | 1:B:467:THR:HG22 | 2.40 | 0.44 |
| 1:B:79:GLY:O | 1:B:80:PHE:CB | 2.65 | 0.44 |
| 1:C:341:LEU:HD23 | 1:C:341:LEU:HA | 1.72 | 0.44 |
| 1:A:146:PHE:HB3 | 1:A:150:MET:HE3 | 1.99 | 0.44 |
| 1:A:410:THR:HG23 | 1:A:411:VAL:N | 2.32 | 0.44 |
| 1:A:444:LEU:HD13 | 1:A:450:GLY:O | 2.17 | 0.44 |
| 1:A:65:PRO:HA | 1:A:68:VAL:CG1 | 2.48 | 0.44 |
| 1:B:322:VAL:HG23 | 1:B:323:VAL:H | 1.82 | 0.44 |
| 1:C:260:GLN:OE1 | 1:C:461:LEU:CD2 | 2.59 | 0.44 |
| 1:C:187:PHE:HA | 1:C:340:TYR:HE1 | 1.83 | 0.44 |
| 1:C:452:ILE:O | 1:C:456:ILE:HG13 | 2.18 | 0.44 |
| 1:A:187:PHE:CE1 | 1:A:347:MET:HB2 | 2.53 | 0.44 |
| 1:A:444:LEU:C | 1:A:446:ALA:H | 2.19 | 0.44 |
| 1:B:82:ASP:O | 1:B:86:ASN:OD1 | 2.35 | 0.44 |
| 1:C:502:ILE:O | 1:C:506:LEU:HD13 | 2.18 | 0.44 |
| 1:B:188:HIS:CD2 | 1:B:367:THR:HA | 2.53 | 0.43 |
| 1:B:399:LEU:HD12 | 1:B:400:GLY:N | 2.33 | 0.43 |
| 1:C:271:ILE:HD13 | 1:C:276:ASP:OD2 | 2.18 | 0.43 |
| 1:C:491:VAL:HG13 | 1:C:492:THR:N | 2.33 | 0.43 |
| 1:B:99:LEU:O | 1:B:102:ALA:HB3 | 2.19 | 0.43 |
| 1:B:222:VAL:O | 1:B:223:PRO:C | 2.54 | 0.43 |
| 1:B:248:PHE:HA | 1:B:251:ALA:HB3 | 2.00 | 0.43 |
| 1:C:232:GLY:O | 1:C:233:TRP:C | 2.55 | 0.43 |
| 1:C:70:VAL:HG13 | 1:C:71:LEU:HD23 | 1.99 | 0.43 |
| 1:A:214:LYS:HG3 | 1:A:219:SER:OG | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:110:PHE:O | 1:B:114:ILE:HG12 | 2.17 | 0.43 |
| 1:B:222:VAL:HB | 1:B:223:PRO:HD3 | 2.00 | 0.43 |
| 1:B:284:SER:O | 1:B:288:LEU:HB2 | 2.18 | 0.43 |
| 1:B:166:TYR:CD1 | 1:B:421:ILE:HG23 | 2.54 | 0.43 |
| 1:B:127:LEU:HD23 | 1:B:127:LEU:C | 2.39 | 0.43 |
| 1:B:189:TRP:CZ2 | 1:B:370:TYR:OH | 2.68 | 0.43 |
| 1:B:432:GLY:O | 1:B:434:GLY:N | 2.47 | 0.43 |
| 1:C:154:LEU:HB3 | 1:C:412:TRP:CD1 | 2.54 | 0.43 |
| 1:C:174:ASP:OD1 | 1:C:174:ASP:O | 2.37 | 0.43 |
| 1:A:353:MET:HE1 | 1:C:328:SER:OG | 2.18 | 0.43 |
| 1:C:189:TRP:CD2 | 1:C:413:PHE:CZ | 3.06 | 0.43 |
| 1:C:159:THR:HG21 | 1:C:443:LEU:HD21 | 1.99 | 0.43 |
| 1:A:130:ILE:O | 1:A:131:ASP:HB3 | 2.17 | 0.43 |
| 1:A:137:ARG:HD2 | 1:A:139:VAL:CG2 | 2.40 | 0.43 |
| 1:A:243:ILE:HG13 | 1:A:243:ILE:H | 1.71 | 0.43 |
| 1:A:288:LEU:HD12 | 1:A:288:LEU:C | 2.39 | 0.43 |
| 1:A:209:PHE:HZ | 1:A:387:ARG:HH12 | 1.64 | 0.43 |
| 1:A:92:LEU:CD1 | 1:A:96:VAL:HG21 | 2.44 | 0.43 |
| 1:B:463:THR:C | 1:B:465:PHE:N | 2.72 | 0.43 |
| 1:C:96:VAL:O | 1:C:100:GLY:HA3 | 2.18 | 0.43 |
| 1:C:187:PHE:CE1 | 1:C:347:MET:HG3 | 2.53 | 0.43 |
| 1:C:484:GLN:HB3 | 1:C:486:GLU:HG2 | 2.00 | 0.43 |
| 1:C:157:TYR:OH | 1:C:519:GLN:NE2 | 2.51 | 0.43 |
| 1:A:124:THR:O | 1:A:125:ILE:C | 2.57 | 0.43 |
| 1:A:155:MET:SD | 1:A:460:LEU:HG | 2.59 | 0.43 |
| 1:A:163:LEU:HD12 | 1:A:163:LEU:HA | 1.75 | 0.43 |
| 1:B:106:PHE:O | 1:B:109:VAL:N | 2.49 | 0.43 |
| 1:B:125:ILE:HG13 | 1:B:125:ILE:H | 1.69 | 0.43 |
| 1:B:159:THR:CG2 | 1:B:443:LEU:HD23 | 2.49 | 0.43 |
| 1:B:554:ARG:HD2 | 1:B:558:ARG:NH2 | 2.34 | 0.43 |
| 1:C:564:ALA:HA | 1:C:567:ARG:HH11 | 1.83 | 0.43 |
| 1:A:190:THR:OG1 | 1:A:191:LEU:N | 2.50 | 0.43 |
| 1:A:393:SER:OG | 1:A:394:ILE:N | 2.52 | 0.43 |
| 1:A:163:LEU:HD22 | 1:A:420:ALA:HB1 | 2.00 | 0.43 |
| 1:A:375:ILE:CG2 | 1:A:529:PHE:HB3 | 2.49 | 0.43 |
| 1:A:558:ARG:HA | 1:A:558:ARG:HH11 | 1.84 | 0.43 |
| 1:B:208:THR:HG21 | 1:B:215:GLN:HA | 2.01 | 0.43 |
| 1:B:220:ALA:O | 1:B:223:PRO:HD2 | 2.18 | 0.43 |
| 1:B:320:VAL:CG2 | 1:B:321:PHE:N | 2.81 | 0.43 |
| 1:C:189:TRP:C | 1:C:193:PRO:HG3 | 2.39 | 0.43 |
| 1:C:257:GLY:O | 1:C:261:ILE:HG12 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:389:SER:O | 1:C:390:ARG:O | 2.36 | 0.43 |
| 1:C:92:LEU:O | 1:C:95:VAL:CG1 | 2.67 | 0.43 |
| 1:A:141:TRP:O | 1:A:144:MET:HB2 | 2.19 | 0.43 |
| 1:A:153:ASP:CA | 1:A:156:PHE:CE2 | 2.74 | 0.43 |
| 1:A:481:GLN:HG3 | 1:A:484:GLN:HG3 | 2.00 | 0.43 |
| 1:A:485:LEU:O | 1:A:486:GLU:O | 2.36 | 0.43 |
| 1:B:375:ILE:CG2 | 1:B:526:ALA:CB | 2.96 | 0.43 |
| 1:B:411:VAL:HG12 | 1:B:412:TRP:N | 2.33 | 0.43 |
| 1:C:178:VAL:HG23 | 1:C:179:GLY:H | 1.84 | 0.43 |
| 1:C:154:LEU:HB3 | 1:C:412:TRP:NE1 | 2.33 | 0.43 |
| 1:C:69:ILE:N | 1:C:69:ILE:CD1 | 2.82 | 0.43 |
| 1:A:182:MET:O | 1:A:186:MET:HG3 | 2.19 | 0.43 |
| 1:A:442:GLY:HA2 | 1:A:445:HIS:CD2 | 2.54 | 0.43 |
| 1:A:442:GLY:HA2 | 1:A:445:HIS:NE2 | 2.34 | 0.43 |
| 1:A:527:THR:HG23 | 1:A:528:PRO:N | 2.33 | 0.43 |
| 1:A:532:VAL:O | 1:A:536:LEU:HB2 | 2.19 | 0.43 |
| 1:B:319:PHE:CE2 | 1:B:453:MET:HG3 | 2.54 | 0.43 |
| 1:C:167:ARG:NH2 | 1:C:424:GLU:OE2 | 2.52 | 0.43 |
| 1:A:453:MET:O | 1:A:456:ILE:N | 2.52 | 0.43 |
| 1:A:544:LEU:C | 1:A:546:ASN:N | 2.73 | 0.43 |
| 1:A:92:LEU:HA | 1:A:95:VAL:HG22 | 1.99 | 0.43 |
| 1:B:145:MET:HE3 | 1:B:404:VAL:HG21 | 2.01 | 0.43 |
| 1:B:309:ASN:CG | 1:B:463:THR:HG23 | 2.39 | 0.43 |
| 1:C:190:THR:C | 1:C:193:PRO:HD2 | 2.40 | 0.43 |
| 1:C:186:MET:CE | 1:C:410:THR:HG1 | 2.31 | 0.43 |
| 1:A:170:VAL:HG13 | 1:A:171:PRO:CD | 2.49 | 0.42 |
| 1:A:209:PHE:HE2 | 1:A:386:ALA:O | 2.02 | 0.42 |
| 1:A:59:ASN:HD21 | 1:A:482:HIS:HA | 1.84 | 0.42 |
| 1:B:291:ILE:HA | 1:B:466:ILE:HD13 | 1.99 | 0.42 |
| 1:B:385:LEU:C | 1:B:385:LEU:HD12 | 2.39 | 0.42 |
| 1:B:123:GLY:O | 1:B:394:ILE:HG13 | 2.18 | 0.42 |
| 1:C:153:ASP:OD1 | 1:C:253:SER:OG | 2.37 | 0.42 |
| 1:C:291:ILE:HD12 | 1:C:469:ALA:HB1 | 2.00 | 0.42 |
| 1:C:559:PHE:C | 1:C:561:ALA:H | 2.23 | 0.42 |
| 1:A:333:LEU:HB3 | 1:A:334:PRO:HD3 | 2.01 | 0.42 |
| 1:A:353:MET:O | 1:A:357:GLY:N | 2.52 | 0.42 |
| 1:A:371:TRP:HE3 | 1:A:371:TRP:N | 2.18 | 0.42 |
| 1:B:321:PHE:CZ | 1:B:326:THR:HG23 | 2.54 | 0.42 |
| 1:B:96:VAL:HG12 | 1:B:96:VAL:O | 2.19 | 0.42 |
| 1:C:170:VAL:HG13 | 1:C:171:PRO:CD | 2.35 | 0.42 |
| 1:A:97:ASP:O | 1:C:327:VAL:HG13 | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:392:ARG:HD2 | 1:C:396:GLU:CD | 2.39 | 0.42 |
| 1:C:414:SER:O | 1:C:418:GLY:CA | 2.63 | 0.42 |
| 1:C:417:GLY:O | 1:C:421:ILE:HG12 | 2.19 | 0.42 |
| 1:A:202:LEU:HD23 | 1:A:202:LEU:HA | 1.85 | 0.42 |
| 1:A:232:GLY:O | 1:A:233:TRP:C | 2.57 | 0.42 |
| 1:A:563:LEU:O | 1:A:563:LEU:HD23 | 2.18 | 0.42 |
| 1:C:78:ILE:HG13 | 1:C:79:GLY:H | 1.84 | 0.42 |
| 1:A:122:PHE:O | 1:A:125:ILE:HB | 2.19 | 0.42 |
| 1:A:353:MET:O | 1:C:178:VAL:HG21 | 2.20 | 0.42 |
| 1:C:193:PRO:HA | 1:C:374:TRP:CD1 | 2.54 | 0.42 |
| 1:C:323:VAL:CG1 | 1:C:324:GLY:N | 2.81 | 0.42 |
| 1:C:371:TRP:CE3 | 1:C:371:TRP:CA | 3.01 | 0.42 |
| 1:C:383:MET:SD | 1:C:475:VAL:HG13 | 2.59 | 0.42 |
| 1:A:157:TYR:HB3 | 1:A:189:TRP:CH2 | 2.53 | 0.42 |
| 1:A:194:TRP:CZ2 | 1:A:405:PRO:HB3 | 2.54 | 0.42 |
| 1:A:152:ILE:CD1 | 1:A:464:PHE:HB3 | 2.49 | 0.42 |
| 1:B:437:GLU:CD | 1:B:437:GLU:H | 2.21 | 0.42 |
| 1:B:92:LEU:O | 1:B:93:SER:C | 2.57 | 0.42 |
| 1:C:154:LEU:N | 1:C:154:LEU:HD12 | 2.34 | 0.42 |
| 1:C:160:THR:HG21 | 1:C:436:ALA:HB1 | 2.00 | 0.42 |
| 1:C:166:TYR:OH | 1:C:425:GLN:HG2 | 2.19 | 0.42 |
| 1:A:152:ILE:N | 1:A:152:ILE:HD12 | 2.33 | 0.42 |
| 1:B:204:ILE:HD11 | 1:B:217:LEU:HA | 2.02 | 0.42 |
| 1:B:122:PHE:CD1 | 1:B:544:LEU:HD13 | 2.55 | 0.42 |
| 1:C:122:PHE:O | 1:C:124:THR:N | 2.53 | 0.42 |
| 1:C:210:ARG:NH2 | 1:C:549:ILE:HD12 | 2.14 | 0.42 |
| 1:C:77:GLY:HA2 | 1:C:85:THR:HB | 2.01 | 0.42 |
| 1:C:134:PRO:HA | 1:C:391:GLY:CA | 2.22 | 0.42 |
| 1:C:337:ILE:O | 1:C:340:TYR:HB3 | 2.20 | 0.42 |
| 1:A:380:PHE:CD2 | 1:A:381:VAL:HG13 | 2.55 | 0.42 |
| 1:A:206:TYR:CE2 | 1:A:544:LEU:HD12 | 2.54 | 0.42 |
| 1:B:152:ILE:HG21 | 1:B:253:SER:O | 2.19 | 0.42 |
| 1:B:265:LEU:HB3 | 1:B:269:ASN:ND2 | 2.35 | 0.42 |
| 1:B:323:VAL:CG2 | 1:B:324:GLY:N | 2.83 | 0.42 |
| 1:B:441:PHE:HA | 1:B:444:LEU:HB2 | 2.01 | 0.42 |
| 1:C:227:GLU:O | 1:C:228:LYS:C | 2.58 | 0.42 |
| 1:A:186:MET:HE3 | 1:A:190:THR:HG21 | 2.02 | 0.42 |
| 1:A:219:SER:O | 1:A:221:PHE:N | 2.53 | 0.42 |
| 1:A:544:LEU:C | 1:A:546:ASN:H | 2.23 | 0.42 |
| 1:B:380:PHE:CE1 | 1:B:471:SER:O | 2.73 | 0.42 |
| 1:C:258:ALA:O | 1:C:261:ILE:HB | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:447:LEU:HB3 | 1:C:448:PRO:HD2 | 2.02 | 0.42 |
| 1:A:213:ARG:HH12 | 1:A:219:SER:C | 2.23 | 0.42 |
| 1:A:354:SER:HA | 1:A:355:ALA:HA | 1.59 | 0.42 |
| 1:A:123:GLY:O | 1:A:393:SER:OG | 2.38 | 0.42 |
| 1:A:461:LEU:O | 1:A:461:LEU:HD12 | 2.20 | 0.42 |
| 1:C:312:LEU:N | 1:C:312:LEU:CD1 | 2.80 | 0.42 |
| 1:C:332:LEU:HA | 1:C:332:LEU:HD23 | 1.81 | 0.42 |
| 1:C:92:LEU:HD12 | 1:C:523:ILE:HG21 | 2.02 | 0.42 |
| 1:A:110:PHE:HD2 | 1:A:196:ILE:CD1 | 2.33 | 0.41 |
| 1:A:256:LEU:HD12 | 1:A:518:LEU:HD21 | 2.02 | 0.41 |
| 1:A:99:LEU:O | 1:A:102:ALA:N | 2.54 | 0.41 |
| 1:B:352:ALA:HB1 | 1:B:360:GLY:HA2 | 2.02 | 0.41 |
| 1:C:521:VAL:O | 1:C:524:VAL:N | 2.53 | 0.41 |
| 1:A:206:TYR:CE2 | 1:A:543:ASP:CG | 2.89 | 0.41 |
| 1:B:109:VAL:O | 1:B:110:PHE:C | 2.59 | 0.41 |
| 1:B:114:ILE:HG13 | 1:B:115:VAL:N | 2.36 | 0.41 |
| 1:B:209:PHE:CD2 | 1:B:390:ARG:HD3 | 2.55 | 0.41 |
| 1:B:406:ALA:O | 1:B:410:THR:HB | 2.18 | 0.41 |
| 1:C:372:ALA:CB | 1:C:523:ILE:HG12 | 2.50 | 0.41 |
| 1:A:216:LEU:HD11 | 1:A:239:ASP:OD2 | 2.21 | 0.41 |
| 1:B:137:ARG:HG3 | 1:B:138:THR:H | 1.85 | 0.41 |
| 1:B:371:TRP:O | 1:B:375:ILE:N | 2.46 | 0.41 |
| 1:B:385:LEU:HD13 | 1:B:397:PHE:CE1 | 2.56 | 0.41 |
| 1:B:557:GLN:HG2 | 1:B:558:ARG:N | 2.35 | 0.41 |
| 1:C:368:ILE:HG23 | 1:C:369:PHE:N | 2.36 | 0.41 |
| 1:A:423:PHE:O | 1:A:428:GLU:N | 2.53 | 0.41 |
| 1:C:234:LEU:HD23 | 1:C:234:LEU:HA | 1.87 | 0.41 |
| 1:C:312:LEU:HB3 | 1:C:460:LEU:HD22 | 2.02 | 0.41 |
| 1:C:401:VAL:O | 1:C:405:PRO:HG2 | 2.19 | 0.41 |
| 1:C:559:PHE:HB2 | 1:C:562:ARG:HE | 1.84 | 0.41 |
| 1:C:76:TRP:O | 1:C:80:PHE:O | 2.39 | 0.41 |
| 1:A:239:ASP:O | 1:A:242:ALA:HB3 | 2.20 | 0.41 |
| 1:B:152:ILE:HG23 | 1:B:153:ASP:N | 2.35 | 0.41 |
| 1:B:216:LEU:C | 1:B:216:LEU:HD23 | 2.40 | 0.41 |
| 1:C:202:LEU:HA | 1:C:202:LEU:HD12 | 1.77 | 0.41 |
| 1:C:203:ALA:HB1 | 1:C:536:LEU:HD11 | 2.03 | 0.41 |
| 1:C:302:ILE:HG23 | 1:C:303:GLN:N | 2.35 | 0.41 |
| 1:C:76:TRP:HD1 | 1:C:77:GLY:CA | 2.33 | 0.41 |
| 1:A:156:PHE:CD1 | 1:A:157:TYR:N | 2.89 | 0.41 |
| 1:B:117:ILE:CG2 | 1:B:398:ILE:HD13 | 2.50 | 0.41 |
| 1:B:132:GLU:HG2 | 1:B:133:ALA:N | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:145:MET:CE | 1:B:404:VAL:CG2 | 2.99 | 0.41 |
| 1:B:444:LEU:HA | 1:B:444:LEU:HD23 | 1.38 | 0.41 |
| 1:B:92:LEU:HD11 | 1:B:523:ILE:CG2 | 2.51 | 0.41 |
| 1:C:134:PRO:HG3 | 1:C:391:GLY:C | 2.39 | 0.41 |
| 1:C:354:SER:HA | 1:C:355:ALA:HA | 1.73 | 0.41 |
| 1:C:453:MET:SD | 1:C:456:ILE:HD12 | 2.61 | 0.41 |
| 1:A:353:MET:HE2 | 1:A:353:MET:CA | 2.40 | 0.41 |
| 1:A:122:PHE:CE1 | 1:A:545:SER:HA | 2.50 | 0.41 |
| 1:B:305:LEU:HD23 | 1:B:467:THR:CG2 | 2.42 | 0.41 |
| 1:B:491:VAL:HG13 | 1:B:492:THR:N | 2.35 | 0.41 |
| 1:C:108:THR:N | 1:C:192:HIS:HE1 | 2.19 | 0.41 |
| 1:A:353:MET:C | 1:A:357:GLY:HA2 | 2.40 | 0.41 |
| 1:A:114:ILE:CD1 | 1:A:402:LEU:HD11 | 2.51 | 0.41 |
| 1:A:98:ASN:O | 1:A:101:TRP:NE1 | 2.49 | 0.41 |
| 1:B:410:THR:HG22 | 1:B:411:VAL:N | 2.35 | 0.41 |
| 1:B:372:ALA:CB | 1:B:523:ILE:HA | 2.50 | 0.41 |
| 1:A:116:VAL:HG22 | 1:A:117:ILE:N | 2.36 | 0.41 |
| 1:A:437:GLU:O | 1:A:441:PHE:CD1 | 2.74 | 0.41 |
| 1:B:209:PHE:CD1 | 1:B:209:PHE:N | 2.89 | 0.41 |
| 1:B:189:TRP:CD2 | 1:B:413:PHE:CZ | 3.09 | 0.41 |
| 1:C:209:PHE:CE1 | 1:C:390:ARG:CB | 3.01 | 0.41 |
| 1:C:463:THR:O | 1:C:467:THR:HG23 | 2.21 | 0.41 |
| 1:C:74:VAL:HG13 | 1:C:502:ILE:HG22 | 2.02 | 0.41 |
| 1:C:81:LYS:CD | 1:C:84:PHE:CD2 | 2.98 | 0.41 |
| 1:A:135:GLU:OE1 | 1:A:136:PHE:CE2 | 2.74 | 0.41 |
| 1:A:331:ASN:C | 1:A:333:LEU:H | 2.24 | 0.41 |
| 1:B:254:LEU:HD12 | 1:B:255:GLY:N | 2.35 | 0.41 |
| 1:C:59:ASN:ND2 | 1:C:62:VAL:CG2 | 2.84 | 0.41 |
| 1:A:383:MET:O | 1:A:387:ARG:NE | 2.54 | 0.41 |
| 1:A:449:GLY:O | 1:A:452:ILE:N | 2.54 | 0.41 |
| 1:A:559:PHE:CE2 | 1:A:563:LEU:CD1 | 2.72 | 0.41 |
| 1:B:352:ALA:CB | 1:B:363:LEU:HD12 | 2.51 | 0.41 |
| 1:B:74:VAL:HG13 | 1:B:75:VAL:N | 2.36 | 0.41 |
| 1:A:334:PRO:HB3 | 1:B:105:LEU:CD1 | 2.51 | 0.40 |
| 1:B:142:ILE:HB | 1:B:145:MET:HE2 | 2.02 | 0.40 |
| 1:B:154:LEU:HD23 | 1:B:154:LEU:N | 2.35 | 0.40 |
| 1:B:372:ALA:O | 1:B:373:TRP:C | 2.57 | 0.40 |
| 1:B:460:LEU:HA | 1:B:463:THR:HG22 | 2.03 | 0.40 |
| 1:C:281:GLY:O | 1:C:285:VAL:CG2 | 2.64 | 0.40 |
| 1:A:200:VAL:HG12 | 1:A:382:GLY:HA3 | 2.03 | 0.40 |
| 1:A:307:ASN:O | 1:A:311:VAL:HG23 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:173:HIS:ND1 | 1:B:180:VAL:HG21 | 2.37 | 0.40 |
| 1:B:95:VAL:CG2 | 1:B:527:THR:HG23 | 2.48 | 0.40 |
| 1:A:581:LYS:O | 1:A:581:LYS:HG2 | 2.22 | 0.40 |
| 1:B:170:VAL:HG11 | 1:B:184:THR:HG21 | 2.02 | 0.40 |
| 1:B:190:THR:O | 1:B:193:PRO:HD2 | 2.21 | 0.40 |
| 1:B:103:PHE:CD1 | 1:B:371:TRP:HB3 | 2.38 | 0.40 |
| 1:B:471:SER:HA | 1:B:474:THR:CG2 | 2.52 | 0.40 |
| 1:B:92:LEU:HD13 | 1:B:523:ILE:HB | 1.95 | 0.40 |
| 1:C:139:VAL:HG13 | 1:C:140:SER:N | 2.37 | 0.40 |
| 1:C:264:GLY:HA2 | 1:C:441:PHE:CD1 | 2.57 | 0.40 |
| 1:C:515:LEU:O | 1:C:518:LEU:HB3 | 2.21 | 0.40 |
| 1:A:191:LEU:HA | 1:A:191:LEU:HD12 | 1.73 | 0.40 |
| 1:B:167:ARG:NH2 | 1:B:431:TRP:CD1 | 2.90 | 0.40 |
| 1:B:214:LYS:HB3 | 1:B:214:LYS:HE2 | 1.82 | 0.40 |
| 1:B:282:ILE:HG13 | 1:B:283:VAL:N | 2.36 | 0.40 |
| 1:C:173:HIS:NE2 | 1:C:180:VAL:HG22 | 2.36 | 0.40 |
| 1:C:295:ILE:HD12 | 1:C:295:ILE:C | 2.42 | 0.40 |
| 1:A:316:LEU:CD1 | 1:A:416:PHE:HZ | 2.34 | 0.40 |
| 1:A:544:LEU:O | 1:A:547:ASP:CB | 2.70 | 0.40 |
| 1:B:385:LEU:O | 1:B:388:ILE:HG22 | 2.22 | 0.40 |
| 1:C:366:TRP:O | 1:C:369:PHE:N | 2.54 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1 | A | 498/566 (88%) | 426 (86%) | 62 (12%) | 10 (2%) | 7 | 33 |
| 1 | B | 470/566 (83%) | 403 (86%) | 61 (13%) | 6 (1%) | 12 | 42 |
| 1 | C | 504/566 (89%) | 435 (86%) | 60 (12%) | 9 (2%) | 8 | 35 |
| All | All | 1472/1698 (87%) | 1264 (86%) | 183 (12%) | 25 (2%) | 9 | 36 |

All (25) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 377 | TRP |
| 1 | A | 403 | LEU |
| 1 | B | 231 | GLU |
| 1 | B | 432 | GLY |
| 1 | C | 231 | GLU |
| 1 | C | 304 | TYR |
| 1 | A | 431 | TRP |
| 1 | A | 486 | GLU |
| 1 | A | 520 | ASN |
| 1 | C | 227 | GLU |
| 1 | C | 232 | GLY |
| 1 | C | 270 | ILE |
| 1 | A | 220 | ALA |
| 1 | A | 302 | ILE |
| 1 | B | 232 | GLY |
| 1 | B | 464 | PHE |
| 1 | C | 429 | SER |
| 1 | A | 388 | ILE |
| 1 | B | 154 | LEU |
| 1 | C | 164 | THR |
| 1 | A | 482 | HIS |
| 1 | B | 545 | SER |
| 1 | C | 325 | PRO |
| 1 | C | 548 | VAL |
| 1 | A | 125 | ILE |

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 | 396/440 (90%) | 378 (96%) | 18 (4%) | 27 | 59 |
| 1 | B | 371/440 (84%) | 356 (96%) | 15 (4%) | 31 | 62 |
| 1 | C | 396/440 (90%) | 369 (93%) | 27 (7%) | 16 | 46 |
| All | All | 1163/1320 (88%) | 1103 (95%) | 60 (5%) | 23 | 55 |

All (60) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 113 | PHE |
| 1 | A | 157 | TYR |
| 1 | A | 189 | TRP |
| 1 | A | 192 | HIS |
| 1 | A | 302 | ILE |
| 1 | A | 344 | PHE |
| 1 | A | 345 | PHE |
| 1 | A | 356 | ASP |
| 1 | A | 371 | TRP |
| 1 | A | 387 | ARG |
| 1 | A | 392 | ARG |
| 1 | A | 424 | GLU |
| 1 | A | 484 | GLN |
| 1 | A | 529 | PHE |
| 1 | A | 542 | LYS |
| 1 | A | 565 | ARG |
| 1 | A | 573 | HIS |
| 1 | A | 574 | ARG |
| 1 | B | 82 | ASP |
| 1 | B | 157 | TYR |
| 1 | B | 177 | ASN |
| 1 | B | 319 | PHE |
| 1 | B | 347 | MET |
| 1 | B | 356 | ASP |
| 1 | B | 366 | TRP |
| 1 | B | 369 | PHE |
| 1 | B | 370 | TYR |
| 1 | B | 371 | TRP |
| 1 | B | 373 | TRP |
| 1 | B | 383 | MET |
| 1 | B | 397 | PHE |
| 1 | B | 444 | LEU |
| 1 | B | 543 | ASP |
| 1 | C | 76 | TRP |
| 1 | C | 92 | LEU |
| 1 | C | 121 | LYS |
| 1 | C | 136 | PHE |
| 1 | C | 144 | MET |
| 1 | C | 153 | ASP |
| 1 | C | 186 | MET |
| 1 | C | 189 | TRP |
| 1 | C | 215 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 218 | SER |
| 1 | C | 304 | TYR |
| 1 | C | 356 | ASP |
| 1 | C | 371 | TRP |
| 1 | C | 374 | TRP |
| 1 | C | 377 | TRP |
| 1 | C | 380 | PHE |
| 1 | C | 387 | ARG |
| 1 | C | 389 | SER |
| 1 | C | 397 | PHE |
| 1 | C | 433 | ASP |
| 1 | C | 437 | GLU |
| 1 | C | 439 | GLN |
| 1 | C | 465 | PHE |
| 1 | C | 468 | SER |
| 1 | C | 481 | GLN |
| 1 | C | 543 | ASP |
| 1 | C | 553 | TYR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 176 | HIS |
| 1 | A | 439 | GLN |
| 1 | A | 484 | GLN |
| 1 | A | 520 | ASN |
| 1 | B | 192 | HIS |
| 1 | B | 215 | GLN |
| 1 | B | 269 | ASN |
| 1 | B | 343 | ASN |
| 1 | B | 426 | ASN |
| 1 | B | 445 | HIS |
| 1 | C | 173 | HIS |
| 1 | C | 176 | HIS |
| 1 | C | 192 | HIS |
| 1 | C | 260 | GLN |
| 1 | C | 339 | ASN |
| 1 | C | 484 | GLN |
| 1 | C | 517 | ASN |
| 1 | C | 519 | GLN |
| 1 | C | 520 | ASN |
| 1 | C | 557 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 2 | CHT | C | 2486 | - | 6,6,6 | 0.78 | 0 | 8,8,8 | 0.26 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|-------|
| 2 | CHT | C | 2486 | - | - | 4/4/4/4 | - |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------|
| 2 | C | 2486 | CHT | C4-C5-N1-C6 |
| 2 | C | 2486 | CHT | C4-C5-N1-C8 |
| 2 | C | 2486 | CHT | C4-C5-N1-C7 |
| 2 | C | 2486 | CHT | O6-C4-C5-N1 |

There are no ring outliers.

1 monomer is involved in 6 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2 | C | 2486 | CHT | 6 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|------------------------------|-----------------------|-------|
| 1 | A | 504/566 (89%) | 0.37 | 44 (8%) 10 12 | 28, 107, 309, 534 | 0 |
| 1 | B | 476/566 (84%) | 0.40 | 47 (9%) 7 8 | 14, 97, 292, 557 | 0 |
| 1 | C | 508/566 (89%) | -0.02 | 20 (3%) 39 41 | 7, 62, 194, 353 | 0 |
| All | All | 1488/1698 (87%) | 0.25 | 111 (7%) 14 16 | 7, 86, 284, 557 | 0 |

All (111) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 296 | SER | 15.2 |
| 1 | B | 296 | SER | 8.9 |
| 1 | A | 297 | GLY | 8.3 |
| 1 | A | 299 | GLY | 7.1 |
| 1 | C | 299 | GLY | 7.0 |
| 1 | B | 500 | ALA | 6.4 |
| 1 | B | 234 | LEU | 6.2 |
| 1 | B | 231 | GLU | 5.8 |
| 1 | B | 499 | THR | 5.6 |
| 1 | C | 228 | LYS | 5.5 |
| 1 | C | 300 | LYS | 5.3 |
| 1 | A | 295 | ILE | 5.0 |
| 1 | B | 393 | SER | 5.0 |
| 1 | C | 301 | GLY | 4.9 |
| 1 | A | 516 | SER | 4.9 |
| 1 | A | 150 | MET | 4.8 |
| 1 | A | 519 | GLN | 4.7 |
| 1 | A | 490 | TRP | 4.7 |
| 1 | A | 83 | SER | 4.7 |
| 1 | B | 80 | PHE | 4.6 |
| 1 | B | 495 | TRP | 4.6 |
| 1 | C | 568 | ARG | 4.6 |
| 1 | B | 551 | LEU | 4.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 140 | SER | 4.4 |
| 1 | B | 492 | THR | 4.3 |
| 1 | B | 298 | VAL | 4.2 |
| 1 | A | 141 | TRP | 4.1 |
| 1 | A | 133 | ALA | 4.1 |
| 1 | A | 300 | LYS | 4.1 |
| 1 | C | 267 | ALA | 4.1 |
| 1 | B | 297 | GLY | 4.0 |
| 1 | B | 496 | GLY | 4.0 |
| 1 | A | 84 | PHE | 4.0 |
| 1 | A | 80 | PHE | 4.0 |
| 1 | B | 249 | GLY | 4.0 |
| 1 | B | 550 | TYR | 3.9 |
| 1 | B | 228 | LYS | 3.9 |
| 1 | B | 71 | LEU | 3.7 |
| 1 | B | 79 | GLY | 3.7 |
| 1 | C | 566 | GLU | 3.7 |
| 1 | B | 150 | MET | 3.6 |
| 1 | B | 227 | GLU | 3.6 |
| 1 | B | 232 | GLY | 3.6 |
| 1 | B | 85 | THR | 3.5 |
| 1 | A | 301 | GLY | 3.5 |
| 1 | A | 142 | ILE | 3.5 |
| 1 | A | 136 | PHE | 3.5 |
| 1 | C | 270 | ILE | 3.4 |
| 1 | A | 388 | ILE | 3.3 |
| 1 | B | 557 | GLN | 3.3 |
| 1 | B | 125 | ILE | 3.3 |
| 1 | B | 558 | ARG | 3.3 |
| 1 | A | 252 | CYS | 3.2 |
| 1 | B | 130 | ILE | 3.2 |
| 1 | B | 252 | CYS | 3.2 |
| 1 | C | 555 | GLU | 3.2 |
| 1 | B | 292 | PHE | 3.2 |
| 1 | A | 228 | LYS | 3.0 |
| 1 | C | 298 | VAL | 3.0 |
| 1 | B | 153 | ASP | 3.0 |
| 1 | B | 62 | VAL | 3.0 |
| 1 | B | 236 | LYS | 2.9 |
| 1 | B | 76 | TRP | 2.9 |
| 1 | B | 255 | GLY | 2.9 |
| 1 | B | 482 | HIS | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 323 | VAL | 2.8 |
| 1 | B | 82 | ASP | 2.8 |
| 1 | A | 227 | GLU | 2.7 |
| 1 | A | 82 | ASP | 2.7 |
| 1 | C | 81 | LYS | 2.7 |
| 1 | A | 292 | PHE | 2.7 |
| 1 | A | 393 | SER | 2.6 |
| 1 | C | 84 | PHE | 2.6 |
| 1 | A | 447 | LEU | 2.6 |
| 1 | B | 61 | SER | 2.6 |
| 1 | C | 268 | ALA | 2.5 |
| 1 | A | 391 | GLY | 2.5 |
| 1 | A | 280 | VAL | 2.5 |
| 1 | A | 294 | ALA | 2.5 |
| 1 | A | 256 | LEU | 2.5 |
| 1 | A | 253 | SER | 2.5 |
| 1 | B | 556 | GLN | 2.5 |
| 1 | A | 298 | VAL | 2.5 |
| 1 | A | 145 | MET | 2.4 |
| 1 | B | 396 | GLU | 2.4 |
| 1 | C | 554 | ARG | 2.4 |
| 1 | C | 278 | THR | 2.4 |
| 1 | B | 386 | ALA | 2.4 |
| 1 | A | 278 | THR | 2.3 |
| 1 | A | 85 | THR | 2.3 |
| 1 | A | 582 | ARG | 2.3 |
| 1 | A | 459 | ILE | 2.3 |
| 1 | B | 391 | GLY | 2.3 |
| 1 | B | 523 | ILE | 2.3 |
| 1 | B | 493 | ALA | 2.2 |
| 1 | B | 295 | ILE | 2.2 |
| 1 | C | 173 | HIS | 2.2 |
| 1 | C | 317 | ALA | 2.2 |
| 1 | B | 226 | GLY | 2.2 |
| 1 | C | 79 | GLY | 2.2 |
| 1 | C | 229 | GLY | 2.2 |
| 1 | B | 138 | THR | 2.2 |
| 1 | A | 287 | THR | 2.1 |
| 1 | A | 230 | ALA | 2.1 |
| 1 | A | 78 | ILE | 2.1 |
| 1 | C | 280 | VAL | 2.1 |
| 1 | A | 60 | TRP | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 146 | PHE | 2.0 |
| 1 | B | 373 | TRP | 2.0 |
| 1 | A | 130 | ILE | 2.0 |
| 1 | A | 448 | PRO | 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2 | CHT | C | 2486 | 7/7 | 0.70 | 0.46 | 85,89,97,97 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.