



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 08:14 am GMT

PDB ID : 2ATC
Title : CRYSTAL AND MOLECULAR STRUCTURES OF NATIVE AND CTP-LIGANDED ASPARTATE CARBAMOYLTRANSFERASE FROM ESCHERICHIA COLI
Authors : Honzatko, R.B.; Crawford, J.L.; Monaco, H.L.; Ladner, J.E.; Edwards, B.F.P.; Evans, D.R.; Warren, S.G.; Wiley, D.C.; Ladner, R.C.; Lipscomb, W.N.
Deposited on : 1982-03-24
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

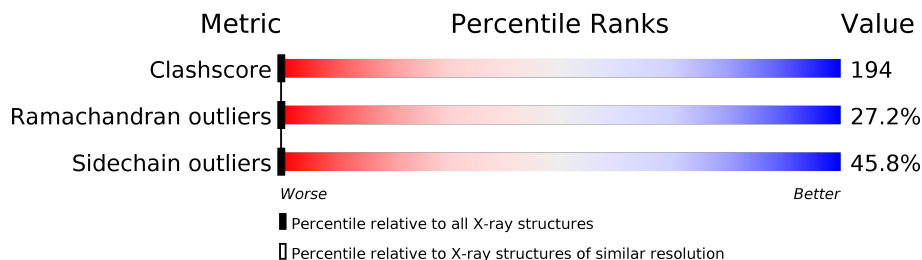
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)) |
|-----------------------|-----------------------------|---|
| Clashscore | 112137 | 2037 (3.00-3.00) |
| Ramachandran outliers | 110173 | 1973 (3.00-3.00) |
| Sidechain outliers | 110143 | 1976 (3.00-3.00) |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 305 | |
| 2 | B | 152 | |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3 | ZN | B | 153 | - | - | X | - |

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3511 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 ASPARTATE CARBAMOYLTRANSFERASE, CATALYTIC CHAIN.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---|---------|---------|-------|
| 1 | A | 305 | Total | C | N | O | S | X | 0 | 0 | 0 |
| | | | 2362 | 1491 | 420 | 441 | 8 | 2 | | | |

There are 25 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| A | 7 | SER | LYS | CONFLICT | UNP P0A786 |
| A | 60 | GLN | GLU | CONFLICT | UNP P0A786 |
| A | 86 | GLN | GLU | CONFLICT | UNP P0A786 |
| A | 90 | ASN | ASP | CONFLICT | UNP P0A786 |
| A | 147 | GLN | GLU | CONFLICT | UNP P0A786 |
| A | 149 | GLU | GLN | CONFLICT | UNP P0A786 |
| A | 153 | ASN | ASP | CONFLICT | UNP P0A786 |
| A | 196 | GLU | GLN | CONFLICT | UNP P0A786 |
| A | ? | - | MET | DELETION | UNP P0A786 |
| A | ? | - | ALA | DELETION | UNP P0A786 |
| A | ? | - | GLU | DELETION | UNP P0A786 |
| A | ? | - | VAL | DELETION | UNP P0A786 |
| A | ? | - | ASP | DELETION | UNP P0A786 |
| A | ? | - | ILE | DELETION | UNP P0A786 |
| A | ? | - | LEU | DELETION | UNP P0A786 |
| A | ? | - | TYR | DELETION | UNP P0A786 |
| A | 234 | ASX | ASN | CONFLICT | UNP P0A786 |
| A | 240 | LEU | VAL | CONFLICT | UNP P0A786 |
| A | 241 | VAL | LEU | CONFLICT | UNP P0A786 |
| A | 244 | ASN | - | INSERTION | UNP P0A786 |
| A | 246 | LEU | - | INSERTION | UNP P0A786 |
| A | 247 | GLY | - | INSERTION | UNP P0A786 |
| A | 248 | GLY | ASP | CONFLICT | UNP P0A786 |
| A | 254 | MET | ALA | CONFLICT | UNP P0A786 |
| A | 256 | ALA | MET | CONFLICT | UNP P0A786 |

- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE, REGULATORY CHAIN.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | B | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1148 | 714 | 202 | 227 | 5 | | | |

There are 17 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| B | 4 | ASN | ASP | CONFLICT | UNP P0A7F3 |
| B | 5 | ASP | ASN | CONFLICT | UNP P0A7F3 |
| B | 10 | ALA | GLU | CONFLICT | UNP P0A7F3 |
| B | 11 | GLU | ALA | CONFLICT | UNP P0A7F3 |
| B | 19 | ASN | ASP | CONFLICT | UNP P0A7F3 |
| B | 24 | GLU | GLN | CONFLICT | UNP P0A7F3 |
| B | 39 | GLN | ASP | CONFLICT | UNP P0A7F3 |
| B | 40 | ASP | GLN | CONFLICT | UNP P0A7F3 |
| B | 70 | GLU | GLN | CONFLICT | UNP P0A7F3 |
| B | 73 | GLU | GLN | CONFLICT | UNP P0A7F3 |
| B | 87 | ASN | ASP | CONFLICT | UNP P0A7F3 |
| B | 88 | ASP | ASN | CONFLICT | UNP P0A7F3 |
| B | 103 | ASN | - | INSERTION | UNP P0A7F3 |
| B | ? | - | ASN | DELETION | UNP P0A7F3 |
| B | 111 | ASP | ASN | CONFLICT | UNP P0A7F3 |
| B | ? | - | LYS | DELETION | UNP P0A7F3 |
| B | 131 | ASP | ASN | CONFLICT | UNP P0A7F3 |

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

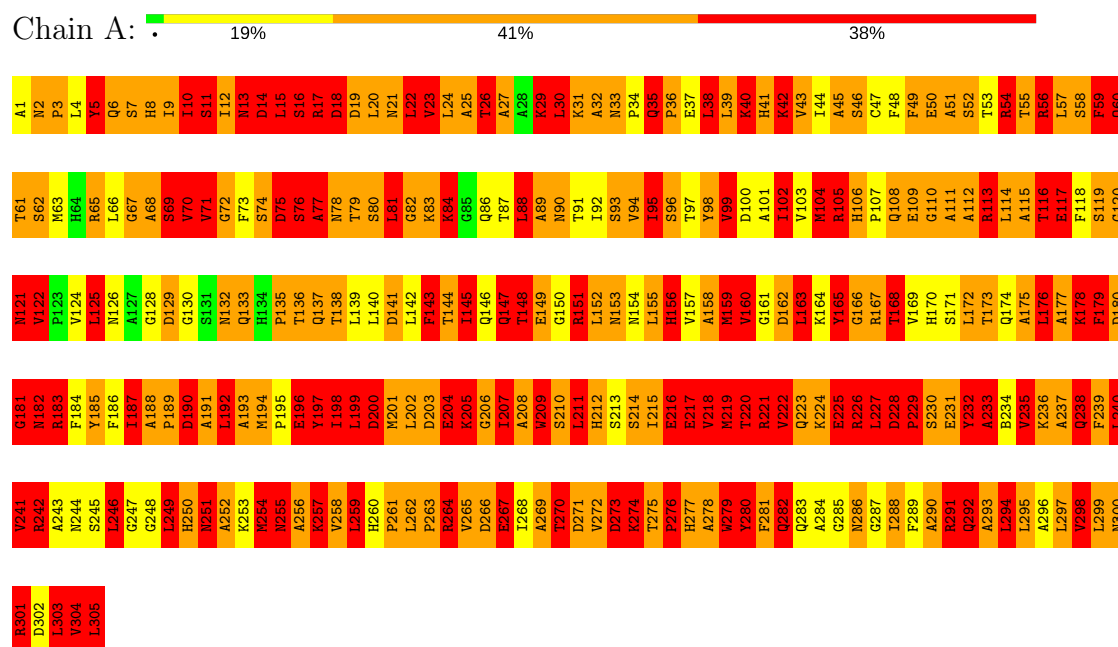
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3 | B | 1 | Total | Zn | 0 | 0 |
| | | | 1 | 1 | | |

3 Residue-property plots

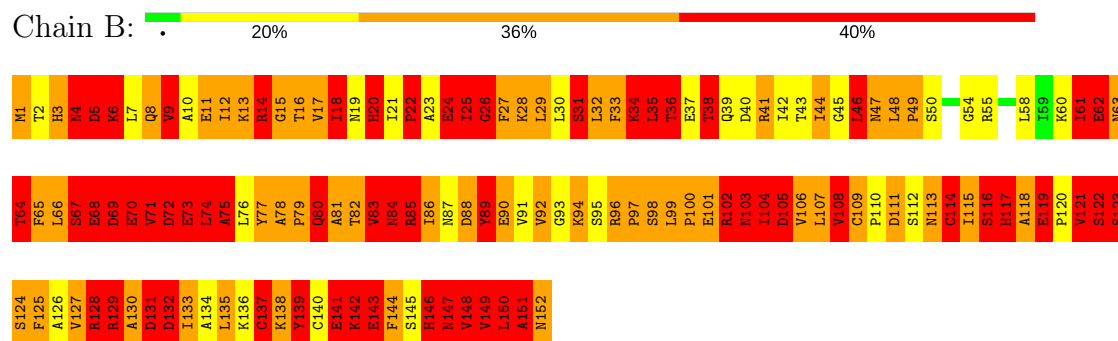
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE, CATALYTIC CHAIN



• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE, REGULATORY CHAIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|--|--|-----------|
| Space group | H 3 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 131.70Å 131.70Å 199.20Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | (Not available) – 3.00 | Depositor |
| % Data completeness (in resolution range) | (Not available) ((Not available)-3.00) | Depositor |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | PROLSQ | Depositor |
| R, R_{free} | 0.270 , (Not available) | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 3511 | wwPDB-VP |
| Average B, all atoms (Å ²) | 49.0 | wwPDB-VP |

5 Model quality

5.1 Standard geometry

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

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 | 1.67 | 28/2399 (1.2%) | 3.68 | 435/3256 (13.4%) |
| 2 | B | 1.80 | 14/1165 (1.2%) | 3.50 | 210/1575 (13.3%) |
| All | All | 1.71 | 42/3564 (1.2%) | 3.62 | 645/4831 (13.4%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 15 |
| 2 | B | 0 | 4 |
| All | All | 0 | 19 |

All (42) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | B | 15 | GLY | N-CA | 13.06 | 1.65 | 1.46 |
| 2 | B | 119 | GLU | CD-OE1 | -8.62 | 1.16 | 1.25 |
| 1 | A | 230 | SER | C-O | 8.43 | 1.39 | 1.23 |
| 1 | A | 230 | SER | N-CA | 7.88 | 1.62 | 1.46 |
| 2 | B | 143 | GLU | CG-CD | -7.51 | 1.40 | 1.51 |
| 2 | B | 129 | ARG | CZ-NH2 | 7.44 | 1.42 | 1.33 |
| 1 | A | 230 | SER | CB-OG | 7.32 | 1.51 | 1.42 |
| 1 | A | 225 | GLU | CD-OE1 | -7.08 | 1.17 | 1.25 |
| 1 | A | 204 | GLU | CD-OE2 | 6.88 | 1.33 | 1.25 |
| 1 | A | 239 | PHE | CA-CB | -6.32 | 1.40 | 1.53 |
| 2 | B | 114 | CYS | CB-SG | -6.11 | 1.71 | 1.82 |
| 1 | A | 11 | SER | CB-OG | -6.04 | 1.34 | 1.42 |
| 2 | B | 64 | THR | C-O | 6.02 | 1.34 | 1.23 |
| 1 | A | 301 | ARG | CZ-NH2 | 5.94 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 301 | ARG | CZ-NH1 | 5.92 | 1.40 | 1.33 |
| 1 | A | 214 | SER | CA-CB | -5.81 | 1.44 | 1.52 |
| 2 | B | 68 | GLU | CD-OE2 | 5.77 | 1.32 | 1.25 |
| 1 | A | 231 | GLU | N-CA | 5.76 | 1.57 | 1.46 |
| 2 | B | 124 | SER | CB-OG | 5.75 | 1.49 | 1.42 |
| 1 | A | 248 | GLY | N-CA | -5.74 | 1.37 | 1.46 |
| 1 | A | 291 | ARG | NE-CZ | -5.66 | 1.25 | 1.33 |
| 1 | A | 264 | ARG | CD-NE | -5.60 | 1.36 | 1.46 |
| 1 | A | 242 | ARG | CZ-NH2 | 5.59 | 1.40 | 1.33 |
| 1 | A | 210 | SER | CA-CB | 5.52 | 1.61 | 1.52 |
| 1 | A | 79 | THR | CB-OG1 | 5.39 | 1.54 | 1.43 |
| 1 | A | 263 | PRO | N-CD | -5.26 | 1.40 | 1.47 |
| 1 | A | 291 | ARG | CD-NE | -5.25 | 1.37 | 1.46 |
| 1 | A | 16 | SER | CA-CB | 5.24 | 1.60 | 1.52 |
| 1 | A | 251 | ASN | N-CA | 5.24 | 1.56 | 1.46 |
| 2 | B | 81 | ALA | N-CA | 5.18 | 1.56 | 1.46 |
| 1 | A | 26 | THR | N-CA | 5.15 | 1.56 | 1.46 |
| 1 | A | 150 | GLY | N-CA | -5.13 | 1.38 | 1.46 |
| 1 | A | 296 | ALA | CA-CB | -5.13 | 1.41 | 1.52 |
| 1 | A | 54 | ARG | CZ-NH2 | 5.13 | 1.39 | 1.33 |
| 2 | B | 54 | GLY | N-CA | 5.13 | 1.53 | 1.46 |
| 2 | B | 38 | THR | CA-CB | 5.11 | 1.66 | 1.53 |
| 1 | A | 82 | GLY | CA-C | 5.09 | 1.59 | 1.51 |
| 2 | B | 112 | SER | CB-OG | 5.09 | 1.48 | 1.42 |
| 1 | A | 181 | GLY | C-O | 5.08 | 1.31 | 1.23 |
| 1 | A | 242 | ARG | CZ-NH1 | 5.06 | 1.39 | 1.33 |
| 2 | B | 93 | GLY | C-O | 5.04 | 1.31 | 1.23 |
| 2 | B | 116 | SER | C-O | 5.00 | 1.32 | 1.23 |

All (645) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | A | 301 | ARG | CD-NE-CZ | 26.04 | 160.05 | 123.60 |
| 1 | A | 242 | ARG | NE-CZ-NH1 | 23.78 | 132.19 | 120.30 |
| 1 | A | 242 | ARG | CD-NE-CZ | 21.68 | 153.95 | 123.60 |
| 1 | A | 54 | ARG | NE-CZ-NH2 | -20.02 | 110.29 | 120.30 |
| 1 | A | 305 | LEU | CA-CB-CG | 19.93 | 161.14 | 115.30 |
| 1 | A | 197 | TYR | CB-CG-CD1 | -19.88 | 109.07 | 121.00 |
| 1 | A | 167 | ARG | NE-CZ-NH2 | 18.97 | 129.79 | 120.30 |
| 1 | A | 197 | TYR | CB-CG-CD2 | 18.89 | 132.34 | 121.00 |
| 1 | A | 147 | GLN | CA-CB-CG | 18.81 | 154.79 | 113.40 |
| 1 | A | 291 | ARG | CD-NE-CZ | 18.65 | 149.70 | 123.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | A | 54 | ARG | CD-NE-CZ | 17.69 | 148.37 | 123.60 |
| 2 | B | 72 | ASP | CB-CG-OD1 | -17.45 | 102.59 | 118.30 |
| 1 | A | 105 | ARG | NE-CZ-NH1 | 17.21 | 128.91 | 120.30 |
| 2 | B | 16 | THR | N-CA-CB | 17.12 | 142.82 | 110.30 |
| 1 | A | 54 | ARG | NE-CZ-NH1 | 16.51 | 128.55 | 120.30 |
| 2 | B | 131 | ASP | CA-CB-CG | 16.16 | 148.96 | 113.40 |
| 1 | A | 292 | GLN | CA-CB-CG | 15.59 | 147.69 | 113.40 |
| 1 | A | 167 | ARG | CD-NE-CZ | 15.48 | 145.27 | 123.60 |
| 2 | B | 14 | ARG | NE-CZ-NH2 | 15.22 | 127.91 | 120.30 |
| 1 | A | 221 | ARG | NE-CZ-NH2 | 14.87 | 127.74 | 120.30 |
| 1 | A | 226 | ARG | NE-CZ-NH1 | 14.81 | 127.71 | 120.30 |
| 1 | A | 149 | GLU | C-N-CA | 14.71 | 153.19 | 122.30 |
| 1 | A | 113 | ARG | NE-CZ-NH1 | -13.44 | 113.58 | 120.30 |
| 2 | B | 132 | ASP | CB-CG-OD1 | 13.41 | 130.37 | 118.30 |
| 1 | A | 203 | ASP | CB-CG-OD1 | 13.29 | 130.26 | 118.30 |
| 2 | B | 118 | ALA | CB-CA-C | 13.13 | 129.80 | 110.10 |
| 1 | A | 225 | GLU | OE1-CD-OE2 | 13.10 | 139.02 | 123.30 |
| 2 | B | 128 | ARG | NE-CZ-NH1 | 13.03 | 126.81 | 120.30 |
| 2 | B | 117 | HIS | CA-CB-CG | 13.02 | 135.73 | 113.60 |
| 1 | A | 204 | GLU | CB-CG-CD | 12.92 | 149.08 | 114.20 |
| 1 | A | 264 | ARG | CD-NE-CZ | 12.89 | 141.65 | 123.60 |
| 1 | A | 105 | ARG | NE-CZ-NH2 | -12.86 | 113.87 | 120.30 |
| 2 | B | 139 | TYR | CB-CG-CD1 | -12.80 | 113.32 | 121.00 |
| 1 | A | 212 | HIS | CA-CB-CG | -12.80 | 91.84 | 113.60 |
| 1 | A | 250 | HIS | CB-CA-C | 12.72 | 135.84 | 110.40 |
| 1 | A | 292 | GLN | CB-CG-CD | 12.67 | 144.53 | 111.60 |
| 1 | A | 38 | LEU | O-C-N | 12.53 | 142.75 | 122.70 |
| 2 | B | 149 | VAL | O-C-N | 12.29 | 142.36 | 122.70 |
| 1 | A | 301 | ARG | NE-CZ-NH1 | 12.18 | 126.39 | 120.30 |
| 1 | A | 125 | LEU | CB-CA-C | 12.16 | 133.30 | 110.20 |
| 2 | B | 129 | ARG | NE-CZ-NH1 | 12.13 | 126.36 | 120.30 |
| 1 | A | 226 | ARG | N-CA-CB | -12.06 | 88.89 | 110.60 |
| 1 | A | 267 | GLU | OE1-CD-OE2 | 11.73 | 137.38 | 123.30 |
| 1 | A | 43 | VAL | CA-C-N | 11.62 | 142.77 | 117.20 |
| 1 | A | 204 | GLU | CA-CB-CG | 11.54 | 138.79 | 113.40 |
| 1 | A | 249 | LEU | N-CA-CB | 11.41 | 133.23 | 110.40 |
| 1 | A | 162 | ASP | CB-CG-OD2 | -11.27 | 108.15 | 118.30 |
| 1 | A | 56 | ARG | CD-NE-CZ | -11.25 | 107.85 | 123.60 |
| 2 | B | 81 | ALA | CB-CA-C | 11.15 | 126.82 | 110.10 |
| 1 | A | 152 | LEU | C-N-CA | 11.14 | 149.56 | 121.70 |
| 1 | A | 225 | GLU | CG-CD-OE2 | -11.11 | 96.08 | 118.30 |
| 1 | A | 296 | ALA | CB-CA-C | 11.11 | 126.76 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | A | 33 | ASN | N-CA-CB | -10.69 | 91.35 | 110.60 |
| 1 | A | 220 | THR | O-C-N | 10.65 | 139.74 | 122.70 |
| 1 | A | 271 | ASP | CA-CB-CG | 10.64 | 136.81 | 113.40 |
| 2 | B | 143 | GLU | CB-CG-CD | 10.59 | 142.78 | 114.20 |
| 1 | A | 243 | ALA | N-CA-CB | -10.58 | 95.29 | 110.10 |
| 1 | A | 232 | TYR | CB-CG-CD1 | 10.56 | 127.33 | 121.00 |
| 1 | A | 270 | THR | CA-CB-CG2 | 10.50 | 127.10 | 112.40 |
| 1 | A | 226 | ARG | CB-CA-C | 10.47 | 131.34 | 110.40 |
| 1 | A | 220 | THR | N-CA-CB | 10.42 | 130.11 | 110.30 |
| 1 | A | 242 | ARG | N-CA-CB | 10.40 | 129.33 | 110.60 |
| 2 | B | 103 | ASN | CA-CB-CG | -10.40 | 90.51 | 113.40 |
| 1 | A | 227 | LEU | CA-C-N | 10.40 | 140.08 | 117.20 |
| 1 | A | 217 | GLU | N-CA-CB | 10.34 | 129.22 | 110.60 |
| 1 | A | 247 | GLY | C-N-CA | 10.28 | 143.89 | 122.30 |
| 1 | A | 196 | GLU | O-C-N | 10.25 | 139.10 | 122.70 |
| 1 | A | 112 | ALA | N-CA-CB | 10.14 | 124.29 | 110.10 |
| 1 | A | 67 | GLY | CA-C-N | 10.09 | 139.39 | 117.20 |
| 1 | A | 210 | SER | N-CA-CB | -10.08 | 95.37 | 110.50 |
| 1 | A | 144 | THR | OG1-CB-CG2 | 10.06 | 133.15 | 110.00 |
| 2 | B | 72 | ASP | CB-CG-OD2 | 10.06 | 127.35 | 118.30 |
| 1 | A | 273 | ASP | CB-CG-OD1 | 10.04 | 127.34 | 118.30 |
| 1 | A | 102 | ILE | CA-C-O | -10.02 | 99.06 | 120.10 |
| 1 | A | 116 | THR | N-CA-CB | 9.91 | 129.12 | 110.30 |
| 2 | B | 6 | LYS | CA-C-N | -9.90 | 95.41 | 117.20 |
| 2 | B | 139 | TYR | CB-CG-CD2 | 9.89 | 126.93 | 121.00 |
| 1 | A | 143 | PHE | CA-C-O | 9.88 | 140.84 | 120.10 |
| 1 | A | 109 | GLU | OE1-CD-OE2 | -9.86 | 111.47 | 123.30 |
| 1 | A | 57 | LEU | CB-CA-C | 9.82 | 128.85 | 110.20 |
| 1 | A | 200 | ASP | CB-CG-OD2 | -9.82 | 109.47 | 118.30 |
| 2 | B | 48 | LEU | CA-CB-CG | 9.81 | 137.86 | 115.30 |
| 2 | B | 61 | ILE | C-N-CA | 9.78 | 146.16 | 121.70 |
| 1 | A | 26 | THR | CA-CB-OG1 | -9.78 | 88.47 | 109.00 |
| 1 | A | 204 | GLU | OE1-CD-OE2 | -9.72 | 111.64 | 123.30 |
| 1 | A | 205 | LYS | CA-CB-CG | 9.68 | 134.69 | 113.40 |
| 1 | A | 1 | ALA | N-CA-CB | -9.67 | 96.57 | 110.10 |
| 2 | B | 81 | ALA | N-CA-CB | -9.66 | 96.58 | 110.10 |
| 2 | B | 103 | ASN | CA-C-N | -9.63 | 96.01 | 117.20 |
| 1 | A | 25 | ALA | N-CA-CB | 9.57 | 123.50 | 110.10 |
| 2 | B | 14 | ARG | NH1-CZ-NH2 | -9.53 | 108.92 | 119.40 |
| 1 | A | 288 | ILE | N-CA-CB | 9.52 | 132.69 | 110.80 |
| 2 | B | 149 | VAL | CA-C-N | -9.48 | 96.35 | 117.20 |
| 1 | A | 180 | ASP | CB-CG-OD1 | -9.47 | 109.78 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 230 | SER | CA-C-N | 9.46 | 138.01 | 117.20 |
| 2 | B | 16 | THR | O-C-N | 9.44 | 137.81 | 122.70 |
| 1 | A | 251 | ASN | CA-C-O | -9.43 | 100.29 | 120.10 |
| 2 | B | 68 | GLU | N-CA-CB | 9.29 | 127.31 | 110.60 |
| 1 | A | 100 | ASP | CB-CG-OD1 | 9.26 | 126.64 | 118.30 |
| 1 | A | 18 | ASP | N-CA-CB | -9.26 | 93.93 | 110.60 |
| 2 | B | 32 | LEU | CB-CA-C | 9.24 | 127.75 | 110.20 |
| 1 | A | 204 | GLU | C-N-CA | 9.23 | 144.78 | 121.70 |
| 1 | A | 246 | LEU | C-N-CA | 9.19 | 141.59 | 122.30 |
| 1 | A | 269 | ALA | N-CA-CB | -9.17 | 97.26 | 110.10 |
| 1 | A | 235 | VAL | N-CA-CB | 9.17 | 131.67 | 111.50 |
| 2 | B | 36 | THR | N-CA-CB | 9.17 | 127.72 | 110.30 |
| 2 | B | 141 | GLU | CG-CD-OE2 | -9.10 | 100.09 | 118.30 |
| 2 | B | 33 | PHE | CB-CG-CD1 | -9.09 | 114.44 | 120.80 |
| 2 | B | 68 | GLU | CG-CD-OE1 | 9.09 | 136.47 | 118.30 |
| 2 | B | 150 | LEU | CB-CA-C | 9.08 | 127.45 | 110.20 |
| 1 | A | 292 | GLN | OE1-CD-NE2 | -9.06 | 101.07 | 121.90 |
| 1 | A | 108 | GLN | O-C-N | 9.04 | 137.17 | 122.70 |
| 1 | A | 227 | LEU | CA-C-O | -9.04 | 101.11 | 120.10 |
| 1 | A | 197 | TYR | CB-CA-C | 9.03 | 128.46 | 110.40 |
| 1 | A | 35 | GLN | CA-CB-CG | 9.00 | 133.21 | 113.40 |
| 1 | A | 180 | ASP | CB-CG-OD2 | 8.97 | 126.37 | 118.30 |
| 1 | A | 238 | GLN | CA-CB-CG | 8.96 | 133.11 | 113.40 |
| 2 | B | 119 | GLU | CG-CD-OE2 | -8.96 | 100.38 | 118.30 |
| 1 | A | 256 | ALA | CB-CA-C | -8.89 | 96.76 | 110.10 |
| 1 | A | 302 | ASP | CB-CG-OD2 | -8.88 | 110.31 | 118.30 |
| 1 | A | 269 | ALA | CB-CA-C | -8.87 | 96.79 | 110.10 |
| 1 | A | 43 | VAL | CA-CB-CG2 | 8.86 | 124.19 | 110.90 |
| 1 | A | 5 | TYR | CA-CB-CG | -8.85 | 96.58 | 113.40 |
| 1 | A | 212 | HIS | CB-CA-C | -8.85 | 92.69 | 110.40 |
| 2 | B | 14 | ARG | C-N-CA | -8.83 | 103.77 | 122.30 |
| 2 | B | 117 | HIS | O-C-N | 8.79 | 136.77 | 122.70 |
| 1 | A | 221 | ARG | NE-CZ-NH1 | -8.74 | 115.93 | 120.30 |
| 1 | A | 144 | THR | N-CA-CB | -8.72 | 93.72 | 110.30 |
| 2 | B | 137 | CYS | O-C-N | 8.72 | 136.65 | 122.70 |
| 1 | A | 8 | HIS | CA-CB-CG | -8.67 | 98.86 | 113.60 |
| 1 | A | 43 | VAL | CA-C-O | -8.67 | 101.90 | 120.10 |
| 2 | B | 15 | GLY | CA-C-O | -8.67 | 105.00 | 120.60 |
| 1 | A | 301 | ARG | CG-CD-NE | 8.64 | 129.95 | 111.80 |
| 1 | A | 89 | ALA | O-C-N | 8.64 | 136.52 | 122.70 |
| 1 | A | 239 | PHE | C-N-CA | 8.62 | 143.26 | 121.70 |
| 1 | A | 40 | LYS | CB-CA-C | -8.61 | 93.18 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 239 | PHE | CB-CG-CD2 | -8.60 | 114.78 | 120.80 |
| 2 | B | 141 | GLU | OE1-CD-OE2 | 8.60 | 133.61 | 123.30 |
| 1 | A | 17 | ARG | NE-CZ-NH1 | -8.52 | 116.04 | 120.30 |
| 1 | A | 226 | ARG | NE-CZ-NH2 | -8.51 | 116.05 | 120.30 |
| 2 | B | 72 | ASP | C-N-CA | 8.46 | 142.86 | 121.70 |
| 1 | A | 143 | PHE | CA-C-N | -8.43 | 98.64 | 117.20 |
| 2 | B | 151 | ALA | N-CA-CB | -8.43 | 98.30 | 110.10 |
| 1 | A | 168 | THR | CA-CB-OG1 | -8.41 | 91.33 | 109.00 |
| 1 | A | 98 | TYR | CB-CG-CD2 | 8.40 | 126.04 | 121.00 |
| 1 | A | 15 | LEU | C-N-CA | 8.39 | 142.69 | 121.70 |
| 1 | A | 129 | ASP | CB-CG-OD2 | 8.32 | 125.79 | 118.30 |
| 2 | B | 24 | GLU | N-CA-CB | -8.25 | 95.75 | 110.60 |
| 1 | A | 149 | GLU | CG-CD-OE1 | 8.24 | 134.79 | 118.30 |
| 2 | B | 22 | PRO | N-CA-C | -8.23 | 90.69 | 112.10 |
| 1 | A | 230 | SER | CA-C-O | -8.23 | 102.81 | 120.10 |
| 1 | A | 278 | ALA | CA-C-N | 8.20 | 135.25 | 117.20 |
| 1 | A | 32 | ALA | N-CA-CB | -8.18 | 98.65 | 110.10 |
| 1 | A | 106 | HIS | N-CA-CB | -8.17 | 95.90 | 110.60 |
| 2 | B | 71 | VAL | CG1-CB-CG2 | 8.16 | 123.95 | 110.90 |
| 2 | B | 103 | ASN | C-N-CA | -8.14 | 101.34 | 121.70 |
| 2 | B | 62 | GLU | CB-CA-C | -8.14 | 94.13 | 110.40 |
| 2 | B | 103 | ASN | CB-CG-OD1 | -8.13 | 105.34 | 121.60 |
| 2 | B | 131 | ASP | N-CA-CB | 8.13 | 125.24 | 110.60 |
| 2 | B | 70 | GLU | OE1-CD-OE2 | 8.12 | 133.05 | 123.30 |
| 1 | A | 93 | SER | N-CA-CB | 8.12 | 122.68 | 110.50 |
| 1 | A | 228 | ASP | CB-CG-OD1 | -8.11 | 111.00 | 118.30 |
| 1 | A | 71 | VAL | N-CA-CB | -8.07 | 93.74 | 111.50 |
| 1 | A | 240 | LEU | CA-CB-CG | 8.07 | 133.87 | 115.30 |
| 2 | B | 47 | ASN | O-C-N | 8.04 | 135.57 | 122.70 |
| 2 | B | 24 | GLU | CA-CB-CG | 8.04 | 131.09 | 113.40 |
| 1 | A | 27 | ALA | CB-CA-C | 8.03 | 122.14 | 110.10 |
| 1 | A | 8 | HIS | O-C-N | 8.02 | 135.54 | 122.70 |
| 1 | A | 21 | ASN | CA-CB-CG | 8.02 | 131.05 | 113.40 |
| 1 | A | 77 | ALA | CB-CA-C | 8.02 | 122.13 | 110.10 |
| 2 | B | 80 | GLN | CA-CB-CG | 8.00 | 131.00 | 113.40 |
| 1 | A | 8 | HIS | N-CA-CB | 7.98 | 124.96 | 110.60 |
| 1 | A | 288 | ILE | O-C-N | 7.97 | 135.46 | 122.70 |
| 1 | A | 197 | TYR | N-CA-CB | -7.97 | 96.26 | 110.60 |
| 2 | B | 70 | GLU | C-N-CA | 7.96 | 141.59 | 121.70 |
| 2 | B | 15 | GLY | N-CA-C | -7.95 | 93.23 | 113.10 |
| 2 | B | 126 | ALA | CB-CA-C | 7.94 | 122.01 | 110.10 |
| 1 | A | 50 | GLU | OE1-CD-OE2 | -7.93 | 113.78 | 123.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 77 | ALA | O-C-N | 7.91 | 135.36 | 122.70 |
| 2 | B | 68 | GLU | N-CA-C | -7.89 | 89.68 | 111.00 |
| 2 | B | 117 | HIS | N-CA-CB | 7.87 | 124.76 | 110.60 |
| 1 | A | 242 | ARG | NH1-CZ-NH2 | -7.86 | 110.76 | 119.40 |
| 1 | A | 167 | ARG | NH1-CZ-NH2 | -7.84 | 110.78 | 119.40 |
| 2 | B | 141 | GLU | N-CA-CB | -7.83 | 96.51 | 110.60 |
| 1 | A | 197 | TYR | O-C-N | -7.78 | 110.25 | 122.70 |
| 1 | A | 52 | SER | CB-CA-C | 7.78 | 124.87 | 110.10 |
| 1 | A | 242 | ARG | NE-CZ-NH2 | -7.73 | 116.43 | 120.30 |
| 2 | B | 124 | SER | CB-CA-C | 7.72 | 124.77 | 110.10 |
| 1 | A | 129 | ASP | N-CA-CB | 7.72 | 124.49 | 110.60 |
| 1 | A | 270 | THR | CA-CB-OG1 | -7.72 | 92.79 | 109.00 |
| 1 | A | 237 | ALA | N-CA-C | -7.68 | 90.26 | 111.00 |
| 2 | B | 94 | LYS | N-CA-CB | 7.68 | 124.42 | 110.60 |
| 1 | A | 225 | GLU | CB-CG-CD | -7.67 | 93.48 | 114.20 |
| 1 | A | 250 | HIS | N-CA-CB | -7.67 | 96.79 | 110.60 |
| 1 | A | 11 | SER | C-N-CA | 7.66 | 140.85 | 121.70 |
| 1 | A | 16 | SER | O-C-N | 7.66 | 134.95 | 122.70 |
| 2 | B | 5 | ASP | CB-CG-OD1 | 7.65 | 125.19 | 118.30 |
| 1 | A | 217 | GLU | O-C-N | 7.62 | 134.90 | 122.70 |
| 1 | A | 207 | ILE | N-CA-C | 7.62 | 131.57 | 111.00 |
| 1 | A | 280 | TYR | CB-CG-CD2 | 7.61 | 125.57 | 121.00 |
| 2 | B | 5 | ASP | CA-C-O | 7.61 | 136.08 | 120.10 |
| 1 | A | 145 | ILE | CA-CB-CG1 | -7.61 | 96.55 | 111.00 |
| 1 | A | 219 | MET | CA-CB-CG | 7.60 | 126.22 | 113.30 |
| 1 | A | 221 | ARG | CG-CD-NE | 7.59 | 127.75 | 111.80 |
| 2 | B | 129 | ARG | CD-NE-CZ | 7.59 | 134.23 | 123.60 |
| 1 | A | 238 | GLN | N-CA-CB | 7.58 | 124.25 | 110.60 |
| 1 | A | 242 | ARG | CA-C-N | -7.58 | 100.53 | 117.20 |
| 2 | B | 129 | ARG | NH1-CZ-NH2 | -7.58 | 111.06 | 119.40 |
| 1 | A | 212 | HIS | O-C-N | 7.56 | 134.79 | 122.70 |
| 1 | A | 45 | ALA | CA-C-O | -7.53 | 104.29 | 120.10 |
| 1 | A | 290 | ALA | N-CA-CB | 7.51 | 120.62 | 110.10 |
| 1 | A | 273 | ASP | CB-CG-OD2 | -7.51 | 111.54 | 118.30 |
| 1 | A | 29 | LYS | CB-CA-C | -7.51 | 95.38 | 110.40 |
| 1 | A | 52 | SER | N-CA-CB | -7.50 | 99.26 | 110.50 |
| 1 | A | 264 | ARG | NE-CZ-NH1 | 7.49 | 124.04 | 120.30 |
| 1 | A | 144 | THR | CA-CB-CG2 | -7.47 | 101.94 | 112.40 |
| 1 | A | 90 | ASN | N-CA-C | -7.46 | 90.84 | 111.00 |
| 1 | A | 20 | LEU | CB-CA-C | -7.46 | 96.03 | 110.20 |
| 1 | A | 216 | GLU | N-CA-CB | -7.45 | 97.19 | 110.60 |
| 2 | B | 146 | HIS | CB-CA-C | -7.45 | 95.50 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 230 | SER | N-CA-CB | -7.45 | 99.33 | 110.50 |
| 2 | B | 117 | HIS | CB-CA-C | -7.44 | 95.53 | 110.40 |
| 1 | A | 153 | ASN | N-CA-CB | -7.41 | 97.27 | 110.60 |
| 2 | B | 65 | PHE | CB-CG-CD1 | 7.37 | 125.96 | 120.80 |
| 1 | A | 188 | ALA | N-CA-CB | 7.36 | 120.41 | 110.10 |
| 2 | B | 94 | LYS | CB-CG-CD | 7.36 | 130.74 | 111.60 |
| 2 | B | 147 | ASN | CA-C-N | -7.33 | 101.06 | 117.20 |
| 1 | A | 38 | LEU | CB-CA-C | -7.33 | 96.27 | 110.20 |
| 1 | A | 291 | ARG | NE-CZ-NH1 | 7.32 | 123.96 | 120.30 |
| 1 | A | 67 | GLY | O-C-N | -7.32 | 110.99 | 122.70 |
| 1 | A | 226 | ARG | CD-NE-CZ | -7.31 | 113.36 | 123.60 |
| 2 | B | 4 | ASN | C-N-CA | 7.31 | 139.97 | 121.70 |
| 2 | B | 105 | ASP | CB-CA-C | 7.28 | 124.96 | 110.40 |
| 1 | A | 149 | GLU | CG-CD-OE2 | -7.23 | 103.84 | 118.30 |
| 1 | A | 221 | ARG | CD-NE-CZ | 7.21 | 133.69 | 123.60 |
| 2 | B | 65 | PHE | CB-CG-CD2 | -7.20 | 115.76 | 120.80 |
| 1 | A | 81 | LEU | CA-CB-CG | 7.18 | 131.82 | 115.30 |
| 2 | B | 142 | LYS | N-CA-CB | 7.18 | 123.53 | 110.60 |
| 2 | B | 108 | VAL | CG1-CB-CG2 | 7.18 | 122.39 | 110.90 |
| 2 | B | 18 | ILE | C-N-CA | 7.17 | 139.64 | 121.70 |
| 1 | A | 270 | THR | N-CA-CB | -7.15 | 96.71 | 110.30 |
| 1 | A | 104 | MET | CA-CB-CG | 7.14 | 125.43 | 113.30 |
| 1 | A | 109 | GLU | CA-CB-CG | 7.14 | 129.10 | 113.40 |
| 2 | B | 72 | ASP | CA-CB-CG | -7.13 | 97.71 | 113.40 |
| 1 | A | 106 | HIS | CA-CB-CG | 7.11 | 125.68 | 113.60 |
| 2 | B | 68 | GLU | O-C-N | 7.10 | 134.07 | 122.70 |
| 1 | A | 121 | ASN | CA-CB-CG | 7.10 | 129.02 | 113.40 |
| 2 | B | 78 | ALA | CB-CA-C | 7.05 | 120.68 | 110.10 |
| 1 | A | 155 | LEU | CA-C-O | 7.05 | 134.91 | 120.10 |
| 1 | A | 69 | SER | CB-CA-C | 7.04 | 123.47 | 110.10 |
| 2 | B | 1 | MET | CA-C-O | 7.03 | 134.87 | 120.10 |
| 1 | A | 105 | ARG | CD-NE-CZ | 7.03 | 133.44 | 123.60 |
| 1 | A | 159 | MET | CB-CA-C | 7.02 | 124.43 | 110.40 |
| 2 | B | 46 | LEU | O-C-N | -7.01 | 111.48 | 122.70 |
| 1 | A | 108 | GLN | CA-C-O | -7.01 | 105.38 | 120.10 |
| 1 | A | 280 | TYR | CB-CA-C | 7.00 | 124.39 | 110.40 |
| 2 | B | 46 | LEU | CB-CA-C | 6.99 | 123.48 | 110.20 |
| 1 | A | 200 | ASP | O-C-N | 6.99 | 133.88 | 122.70 |
| 2 | B | 62 | GLU | O-C-N | 6.99 | 133.88 | 122.70 |
| 2 | B | 6 | LYS | N-CA-CB | 6.98 | 123.17 | 110.60 |
| 1 | A | 292 | GLN | CG-CD-OE1 | 6.98 | 135.56 | 121.60 |
| 2 | B | 127 | VAL | CB-CA-C | -6.97 | 98.16 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 5 | TYR | CB-CG-CD2 | -6.96 | 116.83 | 121.00 |
| 1 | A | 224 | LYS | CB-CA-C | 6.95 | 124.30 | 110.40 |
| 1 | A | 94 | VAL | CA-C-O | 6.95 | 134.69 | 120.10 |
| 2 | B | 70 | GLU | CG-CD-OE2 | -6.95 | 104.41 | 118.30 |
| 1 | A | 298 | VAL | O-C-N | -6.94 | 111.60 | 122.70 |
| 1 | A | 152 | LEU | CA-CB-CG | 6.93 | 131.24 | 115.30 |
| 2 | B | 137 | CYS | CA-C-O | -6.93 | 105.55 | 120.10 |
| 2 | B | 37 | GLU | CG-CD-OE1 | 6.92 | 132.15 | 118.30 |
| 2 | B | 84 | ASN | CA-CB-CG | 6.92 | 128.63 | 113.40 |
| 1 | A | 226 | ARG | CB-CG-CD | -6.90 | 93.66 | 111.60 |
| 2 | B | 35 | LEU | CB-CA-C | 6.90 | 123.31 | 110.20 |
| 2 | B | 126 | ALA | N-CA-CB | -6.90 | 100.44 | 110.10 |
| 1 | A | 179 | PHE | N-CA-CB | 6.90 | 123.01 | 110.60 |
| 2 | B | 149 | VAL | N-CA-C | -6.90 | 92.38 | 111.00 |
| 2 | B | 71 | VAL | CB-CA-C | -6.89 | 98.31 | 111.40 |
| 2 | B | 37 | GLU | N-CA-C | -6.88 | 92.42 | 111.00 |
| 1 | A | 77 | ALA | N-CA-CB | 6.88 | 119.73 | 110.10 |
| 1 | A | 237 | ALA | CB-CA-C | 6.88 | 120.42 | 110.10 |
| 1 | A | 228 | ASP | CB-CG-OD2 | 6.84 | 124.46 | 118.30 |
| 1 | A | 192 | LEU | CA-C-O | 6.82 | 134.42 | 120.10 |
| 1 | A | 257 | LYS | CA-CB-CG | 6.82 | 128.40 | 113.40 |
| 2 | B | 151 | ALA | N-CA-C | -6.82 | 92.60 | 111.00 |
| 2 | B | 117 | HIS | C-N-CA | -6.80 | 104.69 | 121.70 |
| 1 | A | 231 | GLU | N-CA-CB | -6.79 | 98.38 | 110.60 |
| 1 | A | 102 | ILE | CA-C-N | 6.78 | 132.12 | 117.20 |
| 1 | A | 144 | THR | CB-CA-C | 6.78 | 129.90 | 111.60 |
| 1 | A | 169 | VAL | C-N-CA | 6.77 | 138.61 | 121.70 |
| 1 | A | 52 | SER | C-N-CA | 6.76 | 138.61 | 121.70 |
| 2 | B | 111 | ASP | CB-CG-OD1 | 6.76 | 124.39 | 118.30 |
| 1 | A | 273 | ASP | N-CA-CB | 6.76 | 122.77 | 110.60 |
| 1 | A | 22 | LEU | CA-CB-CG | 6.75 | 130.82 | 115.30 |
| 1 | A | 25 | ALA | CA-C-O | -6.74 | 105.94 | 120.10 |
| 1 | A | 211 | LEU | O-C-N | -6.74 | 111.92 | 122.70 |
| 2 | B | 31 | SER | CA-C-N | -6.74 | 102.38 | 117.20 |
| 2 | B | 129 | ARG | N-CA-C | 6.74 | 129.18 | 111.00 |
| 1 | A | 98 | TYR | CB-CG-CD1 | -6.72 | 116.97 | 121.00 |
| 1 | A | 126 | ASN | O-C-N | 6.72 | 133.46 | 122.70 |
| 1 | A | 258 | VAL | CA-C-O | -6.72 | 105.98 | 120.10 |
| 1 | A | 5 | TYR | CB-CG-CD1 | 6.72 | 125.03 | 121.00 |
| 1 | A | 259 | LEU | CB-CA-C | -6.69 | 97.48 | 110.20 |
| 1 | A | 206 | GLY | C-N-CA | 6.67 | 138.38 | 121.70 |
| 2 | B | 131 | ASP | CB-CG-OD1 | 6.66 | 124.30 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 200 | ASP | OD1-CG-OD2 | 6.65 | 135.94 | 123.30 |
| 2 | B | 67 | SER | CA-CB-OG | 6.65 | 129.16 | 111.20 |
| 2 | B | 129 | ARG | CB-CA-C | -6.64 | 97.11 | 110.40 |
| 1 | A | 72 | GLY | O-C-N | 6.63 | 133.31 | 122.70 |
| 1 | A | 136 | THR | N-CA-CB | 6.63 | 122.89 | 110.30 |
| 1 | A | 217 | GLU | CA-C-N | -6.63 | 102.62 | 117.20 |
| 2 | B | 34 | LYS | CB-CA-C | -6.63 | 97.14 | 110.40 |
| 1 | A | 196 | GLU | CA-C-O | -6.62 | 106.20 | 120.10 |
| 1 | A | 5 | TYR | CB-CA-C | -6.62 | 97.17 | 110.40 |
| 1 | A | 216 | GLU | CB-CA-C | -6.62 | 97.17 | 110.40 |
| 1 | A | 33 | ASN | CA-CB-CG | -6.61 | 98.86 | 113.40 |
| 1 | A | 69 | SER | O-C-N | -6.56 | 112.20 | 122.70 |
| 2 | B | 103 | ASN | CB-CA-C | -6.56 | 97.28 | 110.40 |
| 1 | A | 122 | VAL | CB-CA-C | 6.55 | 123.85 | 111.40 |
| 2 | B | 119 | GLU | CG-CD-OE1 | 6.55 | 131.40 | 118.30 |
| 1 | A | 209 | TRP | CA-C-N | -6.54 | 102.81 | 117.20 |
| 2 | B | 146 | HIS | N-CA-CB | 6.54 | 122.37 | 110.60 |
| 1 | A | 183 | ARG | CA-C-O | 6.52 | 133.79 | 120.10 |
| 1 | A | 143 | PHE | CA-CB-CG | 6.52 | 129.55 | 113.90 |
| 1 | A | 23 | VAL | CB-CA-C | 6.51 | 123.78 | 111.40 |
| 1 | A | 172 | LEU | CA-CB-CG | -6.51 | 100.32 | 115.30 |
| 1 | A | 73 | PHE | O-C-N | 6.48 | 133.07 | 122.70 |
| 1 | A | 251 | ASN | CA-C-N | 6.45 | 131.39 | 117.20 |
| 1 | A | 160 | VAL | N-CA-CB | -6.44 | 97.32 | 111.50 |
| 1 | A | 17 | ARG | NH1-CZ-NH2 | 6.44 | 126.49 | 119.40 |
| 1 | A | 128 | GLY | O-C-N | -6.44 | 112.39 | 122.70 |
| 2 | B | 127 | VAL | CG1-CB-CG2 | 6.44 | 121.20 | 110.90 |
| 2 | B | 68 | GLU | CG-CD-OE2 | -6.43 | 105.43 | 118.30 |
| 1 | A | 273 | ASP | O-C-N | 6.43 | 132.98 | 122.70 |
| 2 | B | 131 | ASP | CB-CG-OD2 | 6.43 | 124.08 | 118.30 |
| 2 | B | 106 | VAL | CA-CB-CG2 | -6.42 | 101.26 | 110.90 |
| 2 | B | 121 | VAL | O-C-N | 6.42 | 132.98 | 122.70 |
| 1 | A | 237 | ALA | CA-C-N | -6.42 | 103.08 | 117.20 |
| 1 | A | 233 | ALA | CB-CA-C | -6.42 | 100.48 | 110.10 |
| 2 | B | 128 | ARG | NH1-CZ-NH2 | -6.41 | 112.35 | 119.40 |
| 2 | B | 88 | ASP | CB-CA-C | 6.40 | 123.21 | 110.40 |
| 1 | A | 238 | GLN | N-CA-C | -6.40 | 93.72 | 111.00 |
| 1 | A | 43 | VAL | N-CA-CB | -6.40 | 97.42 | 111.50 |
| 2 | B | 110 | PRO | N-CD-CG | -6.40 | 93.60 | 103.20 |
| 1 | A | 49 | PHE | CB-CA-C | 6.39 | 123.18 | 110.40 |
| 1 | A | 148 | THR | O-C-N | 6.39 | 132.93 | 122.70 |
| 2 | B | 16 | THR | N-CA-C | -6.39 | 93.75 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | B | 62 | GLU | OE1-CD-OE2 | 6.39 | 130.97 | 123.30 |
| 1 | A | 299 | LEU | N-CA-C | 6.38 | 128.22 | 111.00 |
| 1 | A | 218 | VAL | N-CA-C | -6.37 | 93.79 | 111.00 |
| 2 | B | 48 | LEU | N-CA-C | -6.37 | 93.81 | 111.00 |
| 1 | A | 114 | LEU | N-CA-CB | 6.36 | 123.12 | 110.40 |
| 1 | A | 35 | GLN | CB-CA-C | -6.35 | 97.70 | 110.40 |
| 1 | A | 238 | GLN | CB-CA-C | 6.35 | 123.11 | 110.40 |
| 1 | A | 70 | VAL | O-C-N | 6.35 | 132.86 | 122.70 |
| 1 | A | 159 | MET | CG-SD-CE | 6.35 | 110.36 | 100.20 |
| 2 | B | 15 | GLY | O-C-N | 6.33 | 132.83 | 122.70 |
| 1 | A | 153 | ASN | CB-CG-ND2 | -6.32 | 101.53 | 116.70 |
| 1 | A | 299 | LEU | N-CA-CB | -6.30 | 97.80 | 110.40 |
| 1 | A | 248 | GLY | CA-C-O | -6.29 | 109.27 | 120.60 |
| 1 | A | 301 | ARG | NH1-CZ-NH2 | -6.28 | 112.49 | 119.40 |
| 1 | A | 207 | ILE | CG1-CB-CG2 | 6.28 | 125.22 | 111.40 |
| 1 | A | 10 | ILE | CB-CA-C | -6.27 | 99.06 | 111.60 |
| 1 | A | 29 | LYS | O-C-N | 6.27 | 132.73 | 122.70 |
| 2 | B | 27 | PHE | N-CA-C | -6.27 | 94.08 | 111.00 |
| 1 | A | 9 | ILE | N-CA-CB | -6.26 | 96.39 | 110.80 |
| 1 | A | 241 | VAL | CB-CA-C | 6.26 | 123.29 | 111.40 |
| 1 | A | 223 | GLN | OE1-CD-NE2 | 6.25 | 136.28 | 121.90 |
| 1 | A | 165 | TYR | CB-CG-CD2 | -6.25 | 117.25 | 121.00 |
| 2 | B | 16 | THR | CA-C-O | -6.25 | 106.98 | 120.10 |
| 2 | B | 151 | ALA | CB-CA-C | -6.24 | 100.73 | 110.10 |
| 2 | B | 62 | GLU | CA-C-N | -6.24 | 103.47 | 117.20 |
| 1 | A | 272 | VAL | CB-CA-C | -6.22 | 99.58 | 111.40 |
| 1 | A | 232 | TYR | CB-CA-C | -6.21 | 97.98 | 110.40 |
| 1 | A | 299 | LEU | O-C-N | -6.21 | 112.77 | 122.70 |
| 2 | B | 89 | TYR | CB-CA-C | 6.21 | 122.81 | 110.40 |
| 2 | B | 122 | SER | CA-C-N | 6.19 | 130.81 | 117.20 |
| 1 | A | 84 | LYS | C-N-CA | 6.18 | 135.29 | 122.30 |
| 1 | A | 242 | ARG | N-CA-C | -6.18 | 94.31 | 111.00 |
| 2 | B | 149 | VAL | CA-CB-CG2 | 6.18 | 120.16 | 110.90 |
| 1 | A | 185 | TYR | O-C-N | 6.17 | 132.57 | 122.70 |
| 2 | B | 131 | ASP | OD1-CG-OD2 | -6.17 | 111.57 | 123.30 |
| 2 | B | 105 | ASP | CB-CG-OD2 | -6.17 | 112.75 | 118.30 |
| 1 | A | 298 | VAL | C-N-CA | 6.16 | 137.10 | 121.70 |
| 1 | A | 67 | GLY | CA-C-O | -6.16 | 109.52 | 120.60 |
| 1 | A | 203 | ASP | C-N-CA | 6.15 | 137.09 | 121.70 |
| 2 | B | 9 | VAL | CA-CB-CG1 | 6.13 | 120.09 | 110.90 |
| 2 | B | 70 | GLU | CA-C-O | 6.12 | 132.96 | 120.10 |
| 1 | A | 71 | VAL | N-CA-C | -6.12 | 94.48 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | B | 34 | LYS | N-CA-CB | -6.12 | 99.59 | 110.60 |
| 1 | A | 200 | ASP | CA-CB-CG | -6.11 | 99.95 | 113.40 |
| 1 | A | 255 | ASN | C-N-CA | 6.10 | 136.95 | 121.70 |
| 1 | A | 269 | ALA | N-CA-C | 6.08 | 127.41 | 111.00 |
| 1 | A | 98 | TYR | N-CA-CB | 6.07 | 121.53 | 110.60 |
| 1 | A | 223 | GLN | CG-CD-OE1 | -6.07 | 109.46 | 121.60 |
| 2 | B | 125 | PHE | CA-C-N | 6.07 | 130.56 | 117.20 |
| 1 | A | 60 | GLN | CA-CB-CG | 6.07 | 126.74 | 113.40 |
| 1 | A | 179 | PHE | CA-C-N | 6.07 | 130.54 | 117.20 |
| 1 | A | 31 | LYS | N-CA-CB | 6.06 | 121.51 | 110.60 |
| 1 | A | 148 | THR | N-CA-CB | 6.05 | 121.79 | 110.30 |
| 2 | B | 6 | LYS | CA-C-O | 6.03 | 132.76 | 120.10 |
| 1 | A | 290 | ALA | CA-C-O | -6.02 | 107.46 | 120.10 |
| 1 | A | 45 | ALA | N-CA-CB | -6.01 | 101.68 | 110.10 |
| 2 | B | 29 | LEU | CA-C-N | -6.01 | 103.97 | 117.20 |
| 1 | A | 19 | ASP | CA-CB-CG | 5.99 | 126.57 | 113.40 |
| 2 | B | 83 | VAL | C-N-CA | 5.99 | 136.67 | 121.70 |
| 1 | A | 65 | ARG | NE-CZ-NH1 | 5.98 | 123.29 | 120.30 |
| 1 | A | 208 | ALA | CB-CA-C | 5.98 | 119.07 | 110.10 |
| 2 | B | 2 | THR | N-CA-CB | -5.97 | 98.95 | 110.30 |
| 1 | A | 3 | PRO | O-C-N | -5.96 | 113.16 | 122.70 |
| 2 | B | 79 | PRO | O-C-N | 5.96 | 132.23 | 122.70 |
| 1 | A | 207 | ILE | N-CA-CB | -5.95 | 97.13 | 110.80 |
| 2 | B | 148 | VAL | N-CA-CB | -5.94 | 98.43 | 111.50 |
| 2 | B | 125 | PHE | CA-C-O | -5.93 | 107.64 | 120.10 |
| 1 | A | 70 | VAL | CA-C-N | -5.93 | 104.15 | 117.20 |
| 1 | A | 73 | PHE | CA-C-O | -5.92 | 107.67 | 120.10 |
| 2 | B | 71 | VAL | N-CA-CB | -5.92 | 98.49 | 111.50 |
| 1 | A | 217 | GLU | CG-CD-OE2 | -5.91 | 106.47 | 118.30 |
| 1 | A | 298 | VAL | CA-C-N | 5.88 | 130.14 | 117.20 |
| 1 | A | 125 | LEU | CB-CG-CD1 | -5.88 | 101.01 | 111.00 |
| 1 | A | 189 | PRO | N-CD-CG | -5.87 | 94.39 | 103.20 |
| 2 | B | 36 | THR | O-C-N | 5.87 | 132.09 | 122.70 |
| 1 | A | 42 | LYS | N-CA-CB | -5.87 | 100.04 | 110.60 |
| 1 | A | 173 | THR | CA-CB-OG1 | -5.87 | 96.68 | 109.00 |
| 1 | A | 59 | PHE | N-CA-CB | 5.85 | 121.13 | 110.60 |
| 2 | B | 75 | ALA | C-N-CA | 5.85 | 136.32 | 121.70 |
| 1 | A | 69 | SER | CA-C-O | 5.84 | 132.37 | 120.10 |
| 1 | A | 95 | ILE | N-CA-CB | -5.84 | 97.37 | 110.80 |
| 1 | A | 178 | LYS | CA-C-O | -5.83 | 107.85 | 120.10 |
| 1 | A | 41 | HIS | N-CA-CB | -5.82 | 100.12 | 110.60 |
| 1 | A | 158 | ALA | N-CA-CB | -5.82 | 101.95 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 84 | LYS | CA-CB-CG | 5.82 | 126.20 | 113.40 |
| 1 | A | 88 | LEU | CA-C-O | -5.82 | 107.88 | 120.10 |
| 1 | A | 175 | ALA | N-CA-CB | 5.82 | 118.24 | 110.10 |
| 2 | B | 103 | ASN | N-CA-CB | 5.82 | 121.07 | 110.60 |
| 1 | A | 281 | PHE | N-CA-CB | 5.81 | 121.06 | 110.60 |
| 1 | A | 192 | LEU | CA-C-N | -5.81 | 104.42 | 117.20 |
| 1 | A | 115 | ALA | CA-C-N | 5.80 | 129.97 | 117.20 |
| 1 | A | 143 | PHE | CB-CG-CD1 | 5.80 | 124.86 | 120.80 |
| 1 | A | 223 | GLN | CA-CB-CG | -5.80 | 100.64 | 113.40 |
| 1 | A | 278 | ALA | CA-C-O | -5.79 | 107.94 | 120.10 |
| 1 | A | 65 | ARG | N-CA-CB | 5.79 | 121.02 | 110.60 |
| 2 | B | 29 | LEU | CB-CG-CD1 | 5.79 | 120.84 | 111.00 |
| 1 | A | 167 | ARG | C-N-CA | 5.79 | 136.17 | 121.70 |
| 1 | A | 229 | PRO | CA-N-CD | -5.79 | 103.40 | 111.50 |
| 1 | A | 207 | ILE | C-N-CA | -5.78 | 107.25 | 121.70 |
| 1 | A | 290 | ALA | CA-C-N | 5.78 | 129.91 | 117.20 |
| 2 | B | 44 | ILE | O-C-N | 5.77 | 133.01 | 123.20 |
| 2 | B | 127 | VAL | N-CA-C | 5.76 | 126.55 | 111.00 |
| 1 | A | 138 | THR | CA-CB-OG1 | -5.75 | 96.92 | 109.00 |
| 1 | A | 89 | ALA | CA-C-N | -5.75 | 104.56 | 117.20 |
| 1 | A | 209 | TRP | CA-C-O | 5.75 | 132.17 | 120.10 |
| 2 | B | 61 | ILE | CA-CB-CG2 | 5.75 | 122.39 | 110.90 |
| 1 | A | 138 | THR | OG1-CB-CG2 | 5.74 | 123.20 | 110.00 |
| 2 | B | 142 | LYS | CD-CE-NZ | -5.74 | 98.50 | 111.70 |
| 1 | A | 165 | TYR | CA-C-N | 5.74 | 127.67 | 116.20 |
| 2 | B | 37 | GLU | CA-C-O | -5.73 | 108.07 | 120.10 |
| 1 | A | 125 | LEU | N-CA-C | -5.72 | 95.56 | 111.00 |
| 1 | A | 90 | ASN | CB-CA-C | 5.72 | 121.83 | 110.40 |
| 1 | A | 303 | LEU | C-N-CA | 5.72 | 135.99 | 121.70 |
| 1 | A | 117 | GLU | CB-CA-C | -5.71 | 98.97 | 110.40 |
| 1 | A | 231 | GLU | O-C-N | 5.71 | 131.84 | 122.70 |
| 2 | B | 69 | ASP | CB-CG-OD1 | -5.71 | 113.16 | 118.30 |
| 2 | B | 70 | GLU | CA-C-N | -5.71 | 104.64 | 117.20 |
| 2 | B | 144 | PHE | CB-CA-C | 5.71 | 121.82 | 110.40 |
| 1 | A | 17 | ARG | NE-CZ-NH2 | -5.71 | 117.45 | 120.30 |
| 1 | A | 217 | GLU | CG-CD-OE1 | 5.70 | 129.69 | 118.30 |
| 1 | A | 56 | ARG | NE-CZ-NH1 | -5.69 | 117.45 | 120.30 |
| 2 | B | 103 | ASN | O-C-N | 5.69 | 131.80 | 122.70 |
| 1 | A | 242 | ARG | CG-CD-NE | 5.68 | 123.73 | 111.80 |
| 1 | A | 138 | THR | CA-CB-CG2 | -5.68 | 104.45 | 112.40 |
| 1 | A | 261 | PRO | N-CD-CG | -5.67 | 94.69 | 103.20 |
| 2 | B | 104 | ILE | CA-CB-CG1 | -5.67 | 100.22 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 304 | VAL | C-N-CA | 5.67 | 135.88 | 121.70 |
| 1 | A | 30 | LEU | CB-CA-C | 5.67 | 120.97 | 110.20 |
| 2 | B | 14 | ARG | NE-CZ-NH1 | 5.67 | 123.13 | 120.30 |
| 2 | B | 151 | ALA | O-C-N | 5.66 | 131.76 | 122.70 |
| 2 | B | 123 | SER | CA-CB-OG | 5.66 | 126.48 | 111.20 |
| 1 | A | 19 | ASP | CB-CA-C | 5.66 | 121.71 | 110.40 |
| 2 | B | 27 | PHE | CA-C-N | -5.65 | 104.78 | 117.20 |
| 1 | A | 249 | LEU | O-C-N | 5.64 | 131.73 | 122.70 |
| 1 | A | 13 | ASN | CB-CG-ND2 | -5.64 | 103.16 | 116.70 |
| 1 | A | 82 | GLY | N-CA-C | -5.64 | 99.01 | 113.10 |
| 1 | A | 117 | GLU | CA-CB-CG | 5.63 | 125.78 | 113.40 |
| 2 | B | 139 | TYR | O-C-N | 5.63 | 131.70 | 122.70 |
| 2 | B | 150 | LEU | CA-CB-CG | 5.63 | 128.24 | 115.30 |
| 1 | A | 25 | ALA | CA-C-N | 5.61 | 129.55 | 117.20 |
| 2 | B | 139 | TYR | CA-CB-CG | -5.61 | 102.73 | 113.40 |
| 2 | B | 35 | LEU | O-C-N | -5.61 | 113.72 | 122.70 |
| 2 | B | 108 | VAL | CA-CB-CG2 | -5.60 | 102.50 | 110.90 |
| 1 | A | 288 | ILE | CA-C-O | -5.59 | 108.36 | 120.10 |
| 1 | A | 291 | ARG | NH1-CZ-NH2 | -5.59 | 113.25 | 119.40 |
| 1 | A | 168 | THR | N-CA-CB | -5.59 | 99.69 | 110.30 |
| 1 | A | 288 | ILE | CA-CB-CG2 | 5.59 | 122.07 | 110.90 |
| 1 | A | 75 | ASP | CB-CG-OD1 | 5.58 | 123.32 | 118.30 |
| 1 | A | 122 | VAL | N-CA-C | -5.58 | 95.93 | 111.00 |
| 1 | A | 175 | ALA | N-CA-C | -5.58 | 95.95 | 111.00 |
| 1 | A | 303 | LEU | CA-C-O | 5.58 | 131.81 | 120.10 |
| 2 | B | 135 | LEU | O-C-N | 5.57 | 131.62 | 122.70 |
| 1 | A | 36 | PRO | N-CA-C | -5.56 | 97.63 | 112.10 |
| 1 | A | 266 | ASP | CA-CB-CG | -5.56 | 101.18 | 113.40 |
| 2 | B | 74 | LEU | CB-CA-C | 5.56 | 120.76 | 110.20 |
| 2 | B | 105 | ASP | CA-CB-CG | -5.55 | 101.19 | 113.40 |
| 1 | A | 7 | SER | CA-CB-OG | -5.54 | 96.23 | 111.20 |
| 1 | A | 274 | LYS | CB-CA-C | -5.54 | 99.32 | 110.40 |
| 2 | B | 123 | SER | O-C-N | -5.53 | 113.86 | 122.70 |
| 2 | B | 136 | LYS | CA-C-N | 5.52 | 129.35 | 117.20 |
| 2 | B | 97 | PRO | N-CA-C | -5.52 | 97.75 | 112.10 |
| 1 | A | 215 | ILE | CA-C-N | -5.52 | 105.07 | 117.20 |
| 2 | B | 94 | LYS | O-C-N | 5.51 | 131.53 | 122.70 |
| 1 | A | 141 | ASP | CB-CA-C | -5.51 | 99.39 | 110.40 |
| 1 | A | 185 | TYR | N-CA-CB | -5.50 | 100.69 | 110.60 |
| 1 | A | 135 | PRO | N-CD-CG | -5.50 | 94.95 | 103.20 |
| 2 | B | 116 | SER | CA-C-N | 5.50 | 129.29 | 117.20 |
| 1 | A | 56 | ARG | NE-CZ-NH2 | -5.50 | 117.55 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 29 | LYS | CA-C-N | -5.49 | 105.12 | 117.20 |
| 1 | A | 221 | ARG | N-CA-C | -5.49 | 96.17 | 111.00 |
| 2 | B | 29 | LEU | N-CA-CB | -5.49 | 99.41 | 110.40 |
| 2 | B | 55 | ARG | O-C-N | 5.48 | 131.46 | 122.70 |
| 1 | A | 126 | ASN | CA-C-O | -5.47 | 108.61 | 120.10 |
| 1 | A | 65 | ARG | CD-NE-CZ | -5.46 | 115.95 | 123.60 |
| 1 | A | 109 | GLU | CG-CD-OE1 | 5.45 | 129.20 | 118.30 |
| 1 | A | 10 | ILE | CA-C-O | -5.44 | 108.67 | 120.10 |
| 1 | A | 167 | ARG | CG-CD-NE | 5.44 | 123.23 | 111.80 |
| 2 | B | 97 | PRO | CA-C-O | -5.44 | 107.15 | 120.20 |
| 1 | A | 257 | LYS | O-C-N | 5.44 | 131.40 | 122.70 |
| 1 | A | 174 | GLN | CA-C-O | -5.43 | 108.69 | 120.10 |
| 2 | B | 103 | ASN | CA-C-O | 5.42 | 131.49 | 120.10 |
| 1 | A | 99 | VAL | CA-C-N | -5.42 | 105.27 | 117.20 |
| 1 | A | 223 | GLN | N-CA-C | 5.42 | 125.63 | 111.00 |
| 1 | A | 69 | SER | N-CA-CB | -5.42 | 102.38 | 110.50 |
| 1 | A | 135 | PRO | CB-CA-C | -5.42 | 98.46 | 112.00 |
| 2 | B | 122 | SER | CA-C-O | -5.41 | 108.74 | 120.10 |
| 1 | A | 1 | ALA | CA-C-O | 5.41 | 131.45 | 120.10 |
| 1 | A | 72 | GLY | CA-C-O | -5.41 | 110.87 | 120.60 |
| 1 | A | 271 | ASP | CB-CA-C | 5.39 | 121.18 | 110.40 |
| 2 | B | 2 | THR | CA-C-O | -5.38 | 108.79 | 120.10 |
| 2 | B | 73 | GLU | N-CA-CB | 5.38 | 120.29 | 110.60 |
| 2 | B | 125 | PHE | CB-CA-C | -5.37 | 99.67 | 110.40 |
| 2 | B | 55 | ARG | N-CA-C | -5.36 | 96.54 | 111.00 |
| 1 | A | 172 | LEU | O-C-N | 5.35 | 131.26 | 122.70 |
| 1 | A | 203 | ASP | OD1-CG-OD2 | -5.35 | 113.14 | 123.30 |
| 1 | A | 33 | ASN | CB-CG-ND2 | -5.34 | 103.88 | 116.70 |
| 2 | B | 6 | LYS | O-C-N | 5.34 | 131.25 | 122.70 |
| 2 | B | 73 | GLU | OE1-CD-OE2 | -5.34 | 116.90 | 123.30 |
| 1 | A | 121 | ASN | CB-CG-ND2 | 5.33 | 129.50 | 116.70 |
| 2 | B | 18 | ILE | N-CA-CB | -5.33 | 98.53 | 110.80 |
| 1 | A | 227 | LEU | N-CA-CB | -5.31 | 99.78 | 110.40 |
| 1 | A | 174 | GLN | O-C-N | 5.31 | 131.20 | 122.70 |
| 1 | A | 145 | ILE | CA-CB-CG2 | 5.30 | 121.50 | 110.90 |
| 1 | A | 200 | ASP | N-CA-C | -5.30 | 96.70 | 111.00 |
| 1 | A | 99 | VAL | O-C-N | 5.29 | 131.17 | 122.70 |
| 1 | A | 208 | ALA | CA-C-O | 5.29 | 131.21 | 120.10 |
| 2 | B | 50 | SER | N-CA-C | -5.29 | 96.72 | 111.00 |
| 2 | B | 29 | LEU | CB-CG-CD2 | -5.29 | 102.01 | 111.00 |
| 1 | A | 52 | SER | O-C-N | -5.28 | 114.25 | 122.70 |
| 1 | A | 240 | LEU | N-CA-C | -5.28 | 96.74 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 89 | ALA | N-CA-C | -5.28 | 96.74 | 111.00 |
| 2 | B | 108 | VAL | N-CA-CB | -5.28 | 99.88 | 111.50 |
| 1 | A | 50 | GLU | CA-CB-CG | 5.28 | 125.01 | 113.40 |
| 1 | A | 250 | HIS | CG-ND1-CE1 | 5.28 | 115.59 | 108.20 |
| 1 | A | 182 | ASN | CB-CA-C | 5.27 | 120.94 | 110.40 |
| 1 | A | 273 | ASP | N-CA-C | -5.27 | 96.78 | 111.00 |
| 1 | A | 180 | ASP | N-CA-C | 5.26 | 125.20 | 111.00 |
| 2 | B | 2 | THR | CA-CB-OG1 | -5.26 | 97.96 | 109.00 |
| 1 | A | 80 | SER | N-CA-CB | 5.25 | 118.38 | 110.50 |
| 1 | A | 209 | TRP | CA-CB-CG | -5.24 | 103.74 | 113.70 |
| 1 | A | 225 | GLU | CA-C-O | 5.24 | 131.10 | 120.10 |
| 2 | B | 95 | SER | CA-C-N | -5.23 | 105.69 | 117.20 |
| 2 | B | 79 | PRO | CA-C-N | -5.23 | 105.70 | 117.20 |
| 1 | A | 130 | GLY | O-C-N | 5.23 | 131.06 | 122.70 |
| 1 | A | 136 | THR | CA-CB-CG2 | -5.23 | 105.08 | 112.40 |
| 2 | B | 106 | VAL | CG1-CB-CG2 | 5.23 | 119.26 | 110.90 |
| 1 | A | 207 | ILE | O-C-N | -5.22 | 114.34 | 122.70 |
| 1 | A | 177 | ALA | CB-CA-C | 5.22 | 117.94 | 110.10 |
| 1 | A | 209 | TRP | N-CA-CB | -5.22 | 101.20 | 110.60 |
| 2 | B | 119 | GLU | CB-CG-CD | -5.22 | 100.11 | 114.20 |
| 1 | A | 181 | GLY | C-N-CA | -5.22 | 108.66 | 121.70 |
| 1 | A | 264 | ARG | NH1-CZ-NH2 | -5.21 | 113.67 | 119.40 |
| 1 | A | 222 | VAL | CA-CB-CG1 | 5.21 | 118.71 | 110.90 |
| 2 | B | 49 | PRO | CA-C-N | -5.20 | 105.76 | 117.20 |
| 1 | A | 295 | LEU | C-N-CA | -5.19 | 108.72 | 121.70 |
| 2 | B | 148 | VAL | CA-C-O | -5.19 | 109.21 | 120.10 |
| 2 | B | 61 | ILE | CA-C-O | 5.18 | 130.99 | 120.10 |
| 1 | A | 158 | ALA | CA-C-O | -5.18 | 109.22 | 120.10 |
| 1 | A | 38 | LEU | CA-C-O | -5.18 | 109.22 | 120.10 |
| 1 | A | 218 | VAL | CG1-CB-CG2 | -5.18 | 102.61 | 110.90 |
| 1 | A | 117 | GLU | OE1-CD-OE2 | 5.18 | 129.51 | 123.30 |
| 1 | A | 249 | LEU | CA-C-N | -5.18 | 105.81 | 117.20 |
| 2 | B | 41 | ARG | N-CA-CB | 5.17 | 119.91 | 110.60 |
| 1 | A | 41 | HIS | CA-C-O | 5.16 | 130.94 | 120.10 |
| 2 | B | 18 | ILE | CA-CB-CG1 | -5.16 | 101.19 | 111.00 |
| 1 | A | 163 | LEU | CB-CA-C | -5.16 | 100.40 | 110.20 |
| 2 | B | 26 | GLY | N-CA-C | -5.16 | 100.20 | 113.10 |
| 1 | A | 228 | ASP | CB-CA-C | 5.16 | 120.71 | 110.40 |
| 1 | A | 128 | GLY | CA-C-N | 5.15 | 128.53 | 117.20 |
| 1 | A | 172 | LEU | CB-CG-CD1 | -5.15 | 102.25 | 111.00 |
| 1 | A | 294 | LEU | CB-CG-CD1 | 5.14 | 119.74 | 111.00 |
| 1 | A | 156 | HIS | N-CA-CB | -5.14 | 101.35 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | B | 112 | SER | O-C-N | 5.14 | 130.92 | 122.70 |
| 1 | A | 6 | GLN | CG-CD-OE1 | -5.13 | 111.34 | 121.60 |
| 1 | A | 154 | ASN | CA-C-N | -5.13 | 105.92 | 117.20 |
| 1 | A | 235 | VAL | CA-CB-CG2 | 5.13 | 118.60 | 110.90 |
| 1 | A | 25 | ALA | CB-CA-C | 5.12 | 117.78 | 110.10 |
| 1 | A | 196 | GLU | CG-CD-OE2 | -5.10 | 108.10 | 118.30 |
| 2 | B | 150 | LEU | N-CA-C | -5.10 | 97.23 | 111.00 |
| 1 | A | 59 | PHE | CB-CG-CD1 | 5.09 | 124.36 | 120.80 |
| 1 | A | 205 | LYS | CD-CE-NZ | -5.09 | 99.99 | 111.70 |
| 2 | B | 80 | GLN | C-N-CA | -5.09 | 108.97 | 121.70 |
| 1 | A | 166 | GLY | O-C-N | -5.08 | 114.57 | 122.70 |
| 2 | B | 103 | ASN | OD1-CG-ND2 | 5.07 | 133.57 | 121.90 |
| 2 | B | 24 | GLU | CA-C-O | 5.07 | 130.75 | 120.10 |
| 1 | A | 9 | ILE | CG1-CB-CG2 | 5.07 | 122.54 | 111.40 |
| 1 | A | 205 | LYS | CB-CG-CD | 5.07 | 124.77 | 111.60 |
| 2 | B | 98 | SER | CA-CB-OG | -5.07 | 97.52 | 111.20 |
| 2 | B | 9 | VAL | CB-CA-C | 5.06 | 121.02 | 111.40 |
| 1 | A | 113 | ARG | CD-NE-CZ | -5.06 | 116.52 | 123.60 |
| 1 | A | 176 | LEU | CB-CA-C | 5.06 | 119.81 | 110.20 |
| 2 | B | 31 | SER | N-CA-CB | -5.06 | 102.91 | 110.50 |
| 2 | B | 67 | SER | O-C-N | 5.06 | 130.79 | 122.70 |
| 1 | A | 52 | SER | CA-C-O | 5.06 | 130.72 | 120.10 |
| 2 | B | 121 | VAL | N-CA-C | 5.06 | 124.65 | 111.00 |
| 1 | A | 279 | TRP | CB-CA-C | 5.05 | 120.51 | 110.40 |
| 2 | B | 37 | GLU | CG-CD-OE2 | -5.05 | 108.19 | 118.30 |
| 2 | B | 115 | ILE | N-CA-CB | 5.05 | 122.41 | 110.80 |
| 1 | A | 15 | LEU | CB-CA-C | 5.05 | 119.79 | 110.20 |
| 1 | A | 202 | LEU | CB-CG-CD2 | -5.05 | 102.42 | 111.00 |
| 1 | A | 122 | VAL | O-C-N | 5.04 | 130.68 | 121.10 |
| 1 | A | 302 | ASP | OD1-CG-OD2 | 5.03 | 132.86 | 123.30 |
| 1 | A | 113 | ARG | NH1-CZ-NH2 | 5.03 | 124.94 | 119.40 |
| 1 | A | 214 | SER | CB-CA-C | 5.03 | 119.66 | 110.10 |
| 1 | A | 231 | GLU | CA-C-O | -5.03 | 109.53 | 120.10 |
| 2 | B | 31 | SER | O-C-N | 5.03 | 130.75 | 122.70 |
| 1 | A | 132 | ASN | CB-CG-OD1 | -5.02 | 111.55 | 121.60 |
| 1 | A | 25 | ALA | C-N-CA | -5.02 | 109.16 | 121.70 |
| 2 | B | 144 | PHE | CA-CB-CG | 5.02 | 125.94 | 113.90 |
| 1 | A | 26 | THR | N-CA-CB | -5.01 | 100.77 | 110.30 |
| 1 | A | 225 | GLU | C-N-CA | -5.01 | 109.17 | 121.70 |
| 2 | B | 142 | LYS | CA-CB-CG | 5.01 | 124.43 | 113.40 |
| 1 | A | 214 | SER | N-CA-CB | 5.01 | 118.02 | 110.50 |
| 2 | B | 61 | ILE | O-C-N | -5.01 | 114.69 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | A | 141 | ASP | CA-CB-CG | -5.01 | 102.38 | 113.40 |
| 1 | A | 8 | HIS | CB-CA-C | -5.00 | 100.39 | 110.40 |
| 1 | A | 243 | ALA | CA-C-N | -5.00 | 106.19 | 117.20 |
| 1 | A | 267 | GLU | C-N-CA | 5.00 | 134.20 | 121.70 |
| 2 | B | 85 | ARG | CA-CB-CG | 5.00 | 124.40 | 113.40 |

There are no chirality outliers.

All (19) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 105 | ARG | Sidechain |
| 1 | A | 113 | ARG | Sidechain |
| 1 | A | 151 | ARG | Sidechain |
| 1 | A | 17 | ARG | Sidechain |
| 1 | A | 183 | ARG | Sidechain |
| 1 | A | 221 | ARG | Sidechain |
| 1 | A | 226 | ARG | Sidechain |
| 1 | A | 242 | ARG | Sidechain |
| 1 | A | 264 | ARG | Sidechain |
| 1 | A | 291 | ARG | Sidechain |
| 1 | A | 301 | ARG | Sidechain |
| 1 | A | 35 | GLN | Sidechain |
| 1 | A | 54 | ARG | Sidechain |
| 1 | A | 56 | ARG | Sidechain |
| 1 | A | 65 | ARG | Sidechain |
| 2 | B | 129 | ARG | Sidechain |
| 2 | B | 14 | ARG | Sidechain |
| 2 | B | 85 | ARG | Sidechain |
| 2 | B | 96 | ARG | Sidechain |

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 | 2362 | 0 | 2360 | 840 | 6 |
| 2 | B | 1148 | 0 | 1114 | 518 | 10 |
| 3 | B | 1 | 0 | 0 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All | 3511 | 0 | 3474 | 1348 | 16 |

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 194.

All (1348) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:66:LEU:H | 2:B:66:LEU:CD1 | 1.34 | 1.38 |
| 2:B:9:VAL:CG1 | 2:B:14:ARG:HA | 1.56 | 1.32 |
| 1:A:282:GLN:HE21 | 1:A:282:GLN:N | 1.23 | 1.32 |
| 2:B:128:ARG:NH1 | 2:B:143:GLU:OE1 | 1.60 | 1.32 |
| 1:A:294:LEU:O | 1:A:298:VAL:HG23 | 1.25 | 1.32 |
| 1:A:251:ASN:O | 1:A:253:LYS:N | 1.60 | 1.31 |
| 1:A:282:GLN:NE2 | 1:A:282:GLN:H | 1.29 | 1.31 |
| 1:A:69:SER:O | 1:A:70:VAL:HG13 | 1.33 | 1.29 |
| 2:B:114:CYS:HB3 | 2:B:116:SER:OG | 1.24 | 1.26 |
| 1:A:231:GLU:HB2 | 1:A:232:TYR:CE2 | 1.68 | 1.26 |
| 1:A:157:VAL:O | 1:A:185:TYR:HD1 | 1.14 | 1.24 |
| 2:B:18:ILE:HG23 | 2:B:62:GLU:OE2 | 1.37 | 1.24 |
| 1:A:108:GLN:O | 1:A:129:ASP:O | 1.56 | 1.24 |
| 1:A:140:LEU:HD13 | 1:A:287:GLY:CA | 1.69 | 1.23 |
| 1:A:157:VAL:O | 1:A:185:TYR:CD1 | 1.93 | 1.22 |
| 1:A:20:LEU:O | 1:A:24:LEU:HB2 | 1.40 | 1.21 |
| 1:A:210:SER:C | 1:A:211:LEU:HD23 | 1.60 | 1.21 |
| 2:B:25:ILE:HD12 | 2:B:25:ILE:O | 1.42 | 1.19 |
| 2:B:66:LEU:HD13 | 2:B:66:LEU:N | 1.46 | 1.19 |
| 2:B:4:ASN:OD1 | 2:B:5:ASP:N | 1.75 | 1.18 |
| 1:A:119:SER:O | 1:A:120:GLY:O | 1.59 | 1.18 |
| 2:B:145:SER:O | 2:B:147:ASN:N | 1.77 | 1.18 |
| 1:A:145:ILE:O | 1:A:145:ILE:HD12 | 1.40 | 1.18 |
| 2:B:27:PHE:CA | 2:B:30:LEU:HD12 | 1.73 | 1.17 |
| 1:A:294:LEU:C | 1:A:298:VAL:HG23 | 1.62 | 1.17 |
| 1:A:59:PHE:O | 1:A:62:SER:HB2 | 1.44 | 1.17 |
| 2:B:22:PRO:HG2 | 2:B:25:ILE:HG23 | 1.22 | 1.16 |
| 1:A:157:VAL:HG11 | 1:A:184:PHE:CD2 | 1.80 | 1.16 |
| 1:A:254:MET:O | 1:A:255:ASN:OD1 | 1.63 | 1.15 |
| 1:A:232:TYR:O | 1:A:234:ASX:XD1 | 1.95 | 1.15 |
| 1:A:187:ILE:H | 1:A:187:ILE:HD13 | 1.10 | 1.14 |
| 1:A:201:MET:HA | 1:A:204:GLU:HB3 | 1.20 | 1.14 |
| 2:B:100:PRO:O | 2:B:101:GLU:HG2 | 1.47 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:104:ILE:O | 2:B:123:SER:O | 1.64 | 1.14 |
| 1:A:264:ARG:NH2 | 1:A:273:ASP:OD1 | 1.81 | 1.14 |
| 1:A:303:LEU:HD11 | 1:A:305:LEU:HA | 1.23 | 1.13 |
| 2:B:71:VAL:HA | 2:B:74:LEU:HD11 | 1.26 | 1.13 |
| 2:B:9:VAL:HG13 | 2:B:14:ARG:CA | 1.79 | 1.13 |
| 1:A:197:TYR:CD1 | 1:A:198:ILE:N | 2.15 | 1.13 |
| 1:A:278:ALA:O | 1:A:279:TRP:CB | 1.95 | 1.13 |
| 2:B:114:CYS:CB | 2:B:116:SER:OG | 1.96 | 1.13 |
| 2:B:61:ILE:HG23 | 2:B:62:GLU:HG2 | 1.29 | 1.13 |
| 2:B:101:GLU:O | 2:B:102:ARG:CB | 1.97 | 1.13 |
| 1:A:216:GLU:O | 1:A:219:MET:HB3 | 1.47 | 1.12 |
| 1:A:210:SER:O | 1:A:211:LEU:HD23 | 1.46 | 1.12 |
| 1:A:303:LEU:HD21 | 1:A:305:LEU:HB3 | 1.31 | 1.12 |
| 1:A:257:LYS:HA | 1:A:277:HIS:HA | 1.16 | 1.12 |
| 1:A:140:LEU:HD13 | 1:A:287:GLY:HA2 | 1.23 | 1.12 |
| 2:B:27:PHE:O | 2:B:30:LEU:HB2 | 1.50 | 1.11 |
| 1:A:56:ARG:CD | 1:A:60:GLN:HE22 | 1.61 | 1.11 |
| 2:B:20:HIS:HD2 | 2:B:22:PRO:O | 1.32 | 1.11 |
| 1:A:274:LYS:HD3 | 1:A:274:LYS:C | 1.69 | 1.10 |
| 1:A:29:LYS:CG | 1:A:30:LEU:H | 1.57 | 1.10 |
| 1:A:40:LYS:HD3 | 1:A:41:HIS:NE2 | 1.65 | 1.10 |
| 1:A:143:PHE:O | 1:A:146:GLN:N | 1.84 | 1.10 |
| 2:B:128:ARG:O | 2:B:134:ALA:HB3 | 1.49 | 1.10 |
| 1:A:198:ILE:O | 1:A:199:LEU:HD12 | 1.52 | 1.10 |
| 2:B:86:ILE:HG12 | 2:B:89:TYR:O | 1.48 | 1.10 |
| 2:B:61:ILE:HB | 2:B:82:THR:O | 1.50 | 1.10 |
| 1:A:219:MET:HG3 | 1:A:219:MET:O | 1.51 | 1.09 |
| 2:B:27:PHE:HA | 2:B:30:LEU:HD12 | 1.28 | 1.09 |
| 2:B:32:LEU:HD21 | 2:B:77:TYR:HE2 | 1.14 | 1.09 |
| 2:B:70:GLU:N | 2:B:71:VAL:HG23 | 1.66 | 1.09 |
| 2:B:71:VAL:HG12 | 2:B:72:ASP:H | 1.06 | 1.09 |
| 2:B:71:VAL:C | 2:B:73:GLU:H | 1.50 | 1.09 |
| 1:A:116:THR:HG22 | 1:A:117:GLU:N | 1.58 | 1.08 |
| 1:A:160:VAL:HG12 | 1:A:187:ILE:HB | 1.09 | 1.08 |
| 1:A:87:THR:O | 1:A:89:ALA:N | 1.87 | 1.08 |
| 1:A:157:VAL:HG11 | 1:A:184:PHE:HD2 | 0.92 | 1.08 |
| 2:B:34:LYS:HG2 | 2:B:35:LEU:H | 0.95 | 1.08 |
| 1:A:272:VAL:O | 1:A:273:ASP:C | 1.89 | 1.08 |
| 2:B:119:GLU:HB3 | 2:B:120:PRO:HD2 | 1.32 | 1.07 |
| 2:B:64:THR:O | 2:B:64:THR:HG22 | 1.45 | 1.07 |
| 1:A:162:ASP:N | 1:A:228:ASP:OD2 | 1.87 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:16:THR:O | 2:B:17:VAL:HG23 | 1.55 | 1.07 |
| 2:B:66:LEU:HD22 | 2:B:67:SER:N | 1.69 | 1.06 |
| 1:A:56:ARG:HG2 | 1:A:60:GLN:NE2 | 1.70 | 1.06 |
| 2:B:150:LEU:O | 2:B:151:ALA:HB2 | 1.50 | 1.06 |
| 1:A:95:ILE:O | 1:A:99:VAL:CG2 | 2.03 | 1.06 |
| 1:A:70:VAL:O | 1:A:71:VAL:HG13 | 1.54 | 1.05 |
| 2:B:61:ILE:HG22 | 2:B:62:GLU:N | 1.71 | 1.05 |
| 2:B:70:GLU:H | 2:B:71:VAL:HG23 | 1.15 | 1.05 |
| 1:A:231:GLU:CB | 1:A:232:TYR:CE2 | 2.38 | 1.05 |
| 1:A:276:PRO:O | 1:A:278:ALA:N | 1.90 | 1.05 |
| 2:B:71:VAL:HA | 2:B:74:LEU:CD1 | 1.85 | 1.05 |
| 2:B:74:LEU:N | 2:B:74:LEU:HD13 | 1.71 | 1.05 |
| 1:A:35:GLN:HG3 | 1:A:38:LEU:HD21 | 1.38 | 1.05 |
| 1:A:229:PRO:HA | 1:A:267:GLU:OE2 | 1.57 | 1.05 |
| 2:B:67:SER:HB3 | 2:B:70:GLU:OE2 | 1.57 | 1.04 |
| 1:A:187:ILE:N | 1:A:187:ILE:HD13 | 1.73 | 1.04 |
| 2:B:71:VAL:O | 2:B:73:GLU:N | 1.90 | 1.03 |
| 2:B:27:PHE:HA | 2:B:30:LEU:CD1 | 1.87 | 1.03 |
| 1:A:228:ASP:HB2 | 1:A:229:PRO:HD3 | 1.07 | 1.03 |
| 1:A:27:ALA:HB2 | 1:A:293:ALA:HB2 | 1.37 | 1.03 |
| 2:B:61:ILE:CG1 | 2:B:82:THR:H | 1.72 | 1.03 |
| 1:A:35:GLN:CA | 1:A:35:GLN:HE21 | 1.62 | 1.03 |
| 1:A:249:LEU:O | 1:A:250:HIS:ND1 | 1.92 | 1.03 |
| 1:A:274:LYS:CD | 1:A:275:THR:N | 2.22 | 1.03 |
| 1:A:187:ILE:N | 1:A:187:ILE:CD1 | 2.21 | 1.02 |
| 2:B:61:ILE:HG13 | 2:B:82:THR:H | 0.90 | 1.02 |
| 1:A:142:LEU:O | 1:A:145:ILE:HG23 | 1.58 | 1.02 |
| 2:B:128:ARG:HH21 | 2:B:128:ARG:HB3 | 1.19 | 1.02 |
| 1:A:29:LYS:HG2 | 1:A:30:LEU:N | 1.72 | 1.01 |
| 2:B:131:ASP:O | 2:B:132:ASP:OD1 | 1.76 | 1.01 |
| 1:A:208:ALA:O | 1:A:209:TRP:HB3 | 1.60 | 1.01 |
| 2:B:33:PHE:O | 2:B:34:LYS:O | 1.78 | 1.01 |
| 1:A:235:VAL:CG2 | 1:A:238:GLN:HB2 | 1.89 | 1.01 |
| 1:A:9:ILE:HB | 1:A:125:LEU:CD1 | 1.90 | 1.01 |
| 1:A:260:HIS:H | 1:A:283:GLN:HE22 | 1.05 | 1.00 |
| 2:B:63:ASN:O | 2:B:64:THR:OG1 | 1.77 | 1.00 |
| 1:A:272:VAL:O | 1:A:273:ASP:O | 1.79 | 1.00 |
| 2:B:119:GLU:CB | 2:B:120:PRO:HD2 | 1.85 | 1.00 |
| 2:B:15:GLY:O | 2:B:64:THR:CG2 | 2.08 | 1.00 |
| 2:B:64:THR:N | 2:B:84:ASN:HD22 | 1.60 | 1.00 |
| 2:B:66:LEU:HD22 | 2:B:67:SER:H | 0.84 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:61:ILE:HG13 | 2:B:82:THR:N | 1.74 | 0.99 |
| 1:A:31:LYS:HE2 | 1:A:289:PHE:CE2 | 1.97 | 0.99 |
| 1:A:29:LYS:HG2 | 1:A:30:LEU:H | 0.87 | 0.99 |
| 2:B:34:LYS:CG | 2:B:35:LEU:H | 1.62 | 0.99 |
| 2:B:86:ILE:HG23 | 2:B:90:GLU:HB2 | 1.40 | 0.99 |
| 1:A:138:THR:HG21 | 1:A:171:SER:CB | 1.91 | 0.99 |
| 1:A:67:GLY:O | 1:A:68:ALA:HB2 | 1.57 | 0.99 |
| 1:A:16:SER:O | 1:A:17:ARG:O | 1.81 | 0.98 |
| 1:A:194:MET:HG2 | 1:A:199:LEU:HD11 | 1.44 | 0.98 |
| 1:A:69:SER:O | 1:A:70:VAL:CG1 | 2.11 | 0.98 |
| 1:A:202:LEU:HD12 | 1:A:207:ILE:HG21 | 1.44 | 0.98 |
| 2:B:128:ARG:NH1 | 2:B:143:GLU:CD | 2.16 | 0.98 |
| 1:A:228:ASP:HB2 | 1:A:229:PRO:CD | 1.92 | 0.98 |
| 1:A:80:SER:O | 1:A:81:LEU:HD12 | 1.63 | 0.98 |
| 1:A:303:LEU:CD1 | 1:A:305:LEU:HA | 1.94 | 0.98 |
| 1:A:31:LYS:HE2 | 1:A:289:PHE:CD2 | 1.98 | 0.98 |
| 1:A:145:ILE:HD12 | 1:A:145:ILE:C | 1.76 | 0.98 |
| 1:A:8:HIS:HB2 | 1:A:10:ILE:HD11 | 1.43 | 0.97 |
| 1:A:10:ILE:HG22 | 1:A:10:ILE:O | 1.60 | 0.97 |
| 2:B:28:LYS:O | 2:B:32:LEU:N | 1.96 | 0.97 |
| 2:B:34:LYS:HG2 | 2:B:35:LEU:N | 1.80 | 0.97 |
| 1:A:191:ALA:O | 1:A:192:LEU:HD13 | 1.63 | 0.97 |
| 2:B:32:LEU:CD2 | 2:B:77:TYR:HE2 | 1.77 | 0.97 |
| 1:A:231:GLU:HB2 | 1:A:232:TYR:CD2 | 1.99 | 0.97 |
| 1:A:81:LEU:HD22 | 1:A:82:GLY:N | 1.78 | 0.97 |
| 2:B:66:LEU:CD2 | 2:B:67:SER:H | 1.76 | 0.97 |
| 1:A:187:ILE:H | 1:A:187:ILE:CD1 | 1.75 | 0.96 |
| 2:B:8:GLN:O | 2:B:9:VAL:HG23 | 1.64 | 0.96 |
| 1:A:31:LYS:NZ | 1:A:147:GLN:OE1 | 1.96 | 0.96 |
| 1:A:43:VAL:HA | 1:A:69:SER:HB2 | 1.48 | 0.96 |
| 2:B:74:LEU:H | 2:B:74:LEU:HD13 | 1.27 | 0.96 |
| 1:A:164:LYS:HD3 | 1:A:165:TYR:CE2 | 1.99 | 0.96 |
| 1:A:5:TYR:HE2 | 1:A:300:ASN:O | 1.49 | 0.95 |
| 2:B:34:LYS:O | 2:B:35:LEU:HG | 1.67 | 0.95 |
| 1:A:5:TYR:O | 1:A:7:SER:N | 1.98 | 0.95 |
| 1:A:56:ARG:CG | 1:A:60:GLN:NE2 | 2.30 | 0.95 |
| 2:B:73:GLU:HA | 2:B:73:GLU:OE1 | 1.66 | 0.95 |
| 1:A:14:ASP:OD1 | 1:A:14:ASP:O | 1.85 | 0.95 |
| 1:A:81:LEU:HD22 | 1:A:82:GLY:H | 1.30 | 0.94 |
| 1:A:303:LEU:HD11 | 1:A:305:LEU:CA | 1.96 | 0.94 |
| 2:B:107:LEU:C | 2:B:108:VAL:HG22 | 1.84 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:261:PRO:O | 1:A:262:LEU:O | 1.85 | 0.94 |
| 1:A:40:LYS:HB3 | 1:A:41:HIS:CD2 | 2.03 | 0.94 |
| 1:A:262:LEU:HB3 | 1:A:263:PRO:HA | 1.50 | 0.94 |
| 1:A:88:LEU:HD22 | 1:A:88:LEU:O | 1.68 | 0.94 |
| 1:A:217:GLU:O | 1:A:218:VAL:HG23 | 1.66 | 0.94 |
| 1:A:279:TRP:O | 1:A:281:PHE:N | 2.01 | 0.94 |
| 1:A:67:GLY:O | 1:A:68:ALA:CB | 2.14 | 0.93 |
| 2:B:128:ARG:HB3 | 2:B:128:ARG:NH2 | 1.83 | 0.93 |
| 2:B:23:ALA:O | 2:B:24:GLU:HB2 | 1.65 | 0.93 |
| 1:A:303:LEU:HD21 | 1:A:305:LEU:CD2 | 1.98 | 0.93 |
| 1:A:92:ILE:O | 1:A:96:SER:OG | 1.85 | 0.93 |
| 2:B:23:ALA:O | 2:B:24:GLU:CB | 2.17 | 0.93 |
| 1:A:214:SER:HB3 | 1:A:216:GLU:HG3 | 1.50 | 0.93 |
| 1:A:202:LEU:CD1 | 1:A:207:ILE:HG21 | 1.97 | 0.93 |
| 2:B:114:CYS:HG | 3:B:153:ZN:ZN | 0.75 | 0.93 |
| 2:B:101:GLU:O | 2:B:102:ARG:HB3 | 1.12 | 0.93 |
| 1:A:44:ILE:O | 1:A:71:VAL:CG2 | 2.17 | 0.92 |
| 1:A:8:HIS:HB2 | 1:A:10:ILE:CD1 | 1.97 | 0.92 |
| 1:A:251:ASN:O | 1:A:253:LYS:CA | 2.17 | 0.92 |
| 1:A:260:HIS:N | 1:A:283:GLN:HE22 | 1.67 | 0.92 |
| 1:A:95:ILE:HG22 | 1:A:96:SER:N | 1.82 | 0.92 |
| 2:B:4:ASN:CG | 2:B:5:ASP:H | 1.70 | 0.92 |
| 1:A:138:THR:HG21 | 1:A:171:SER:HB3 | 1.52 | 0.92 |
| 2:B:20:HIS:CD2 | 2:B:22:PRO:O | 2.21 | 0.92 |
| 1:A:201:MET:HA | 1:A:204:GLU:CB | 2.00 | 0.92 |
| 1:A:49:PHE:HB2 | 1:A:105:ARG:O | 1.68 | 0.91 |
| 1:A:159:MET:HE1 | 1:A:172:LEU:HD23 | 1.49 | 0.91 |
| 1:A:56:ARG:HG2 | 1:A:60:GLN:HE21 | 1.24 | 0.91 |
| 1:A:269:ALA:HB3 | 1:A:272:VAL:HG23 | 1.53 | 0.91 |
| 1:A:274:LYS:HD3 | 1:A:275:THR:N | 1.82 | 0.91 |
| 1:A:201:MET:CA | 1:A:204:GLU:HB3 | 2.00 | 0.91 |
| 1:A:94:VAL:O | 1:A:97:THR:OG1 | 1.89 | 0.91 |
| 1:A:230:SER:C | 1:A:231:GLU:HG2 | 1.91 | 0.91 |
| 1:A:234:ASX:XD1 | 1:A:239:PHE:HE1 | 1.84 | 0.91 |
| 2:B:108:VAL:HG21 | 2:B:152:ASN:HB3 | 1.52 | 0.91 |
| 2:B:38:THR:O | 2:B:38:THR:HG22 | 1.71 | 0.91 |
| 2:B:66:LEU:N | 2:B:66:LEU:CD1 | 2.13 | 0.91 |
| 2:B:32:LEU:HD21 | 2:B:106:VAL:HG21 | 1.50 | 0.91 |
| 2:B:140:CYS:HG | 3:B:153:ZN:ZN | 0.77 | 0.91 |
| 2:B:32:LEU:CD2 | 2:B:106:VAL:HG21 | 2.00 | 0.90 |
| 1:A:235:VAL:HG23 | 1:A:238:GLN:HB2 | 1.52 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:71:VAL:HG12 | 2:B:72:ASP:N | 1.86 | 0.90 |
| 1:A:24:LEU:HD21 | 1:A:142:LEU:HD23 | 1.52 | 0.90 |
| 1:A:110:GLY:HA2 | 2:B:139:TYR:O | 1.70 | 0.90 |
| 2:B:32:LEU:HD21 | 2:B:77:TYR:CE2 | 2.06 | 0.90 |
| 2:B:25:ILE:O | 2:B:25:ILE:CD1 | 2.18 | 0.90 |
| 1:A:197:TYR:O | 1:A:199:LEU:N | 2.04 | 0.90 |
| 2:B:71:VAL:O | 2:B:73:GLU:HB2 | 1.72 | 0.90 |
| 1:A:95:ILE:O | 1:A:99:VAL:HG23 | 1.72 | 0.89 |
| 2:B:18:ILE:CA | 2:B:62:GLU:OE1 | 2.19 | 0.89 |
| 2:B:72:ASP:OD1 | 2:B:98:SER:N | 2.05 | 0.89 |
| 1:A:159:MET:CE | 1:A:172:LEU:HD23 | 2.01 | 0.89 |
| 2:B:22:PRO:HG2 | 2:B:25:ILE:CG2 | 2.01 | 0.89 |
| 2:B:86:ILE:HG23 | 2:B:90:GLU:CB | 2.03 | 0.89 |
| 1:A:281:PHE:O | 1:A:284:ALA:N | 2.04 | 0.89 |
| 2:B:71:VAL:CG1 | 2:B:72:ASP:H | 1.82 | 0.89 |
| 1:A:75:ASP:O | 1:A:76:SER:HB2 | 1.72 | 0.89 |
| 2:B:105:ASP:C | 2:B:105:ASP:OD2 | 2.07 | 0.89 |
| 2:B:64:THR:O | 2:B:64:THR:CG2 | 2.21 | 0.89 |
| 1:A:303:LEU:O | 1:A:303:LEU:HD23 | 1.73 | 0.89 |
| 1:A:70:VAL:C | 1:A:71:VAL:HG22 | 1.87 | 0.89 |
| 2:B:1:MET:CE | 2:B:41:ARG:HH22 | 1.85 | 0.89 |
| 2:B:17:VAL:HG22 | 2:B:43:THR:CB | 2.01 | 0.89 |
| 2:B:15:GLY:O | 2:B:64:THR:HG21 | 1.69 | 0.88 |
| 1:A:303:LEU:HG | 1:A:305:LEU:N | 1.88 | 0.88 |
| 1:A:250:HIS:O | 1:A:251:ASN:C | 2.09 | 0.88 |
| 2:B:17:VAL:HG13 | 2:B:43:THR:HB | 1.55 | 0.88 |
| 1:A:216:GLU:O | 1:A:219:MET:CB | 2.21 | 0.88 |
| 1:A:88:LEU:C | 1:A:88:LEU:HD22 | 1.93 | 0.88 |
| 2:B:61:ILE:CG2 | 2:B:62:GLU:N | 2.30 | 0.88 |
| 1:A:254:MET:C | 1:A:255:ASN:OD1 | 2.10 | 0.88 |
| 2:B:111:ASP:O | 2:B:117:HIS:HE1 | 1.57 | 0.88 |
| 1:A:235:VAL:HG23 | 1:A:238:GLN:N | 1.88 | 0.88 |
| 1:A:293:ALA:O | 1:A:297:LEU:HD12 | 1.74 | 0.88 |
| 1:A:35:GLN:CA | 1:A:35:GLN:NE2 | 2.37 | 0.88 |
| 2:B:18:ILE:HA | 2:B:62:GLU:OE1 | 1.73 | 0.88 |
| 2:B:91:VAL:O | 2:B:92:VAL:HG23 | 1.73 | 0.88 |
| 1:A:29:LYS:HD2 | 1:A:29:LYS:H | 1.37 | 0.87 |
| 1:A:231:GLU:CB | 1:A:232:TYR:CD2 | 2.55 | 0.87 |
| 1:A:294:LEU:C | 1:A:298:VAL:CG2 | 2.43 | 0.87 |
| 2:B:71:VAL:HG13 | 2:B:74:LEU:HD21 | 1.57 | 0.87 |
| 1:A:50:GLU:O | 1:A:51:ALA:O | 1.92 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:56:ARG:HD2 | 1:A:60:GLN:HE22 | 1.40 | 0.87 |
| 2:B:9:VAL:CG1 | 2:B:14:ARG:CA | 2.45 | 0.87 |
| 1:A:152:LEU:HD22 | 1:A:176:LEU:HD21 | 1.54 | 0.87 |
| 2:B:132:ASP:O | 2:B:146:HIS:CE1 | 2.27 | 0.87 |
| 1:A:68:ALA:O | 1:A:69:SER:OG | 1.91 | 0.87 |
| 2:B:86:ILE:O | 2:B:90:GLU:CG | 2.22 | 0.87 |
| 2:B:107:LEU:O | 2:B:108:VAL:HG13 | 1.74 | 0.87 |
| 2:B:9:VAL:HG12 | 2:B:10:ALA:H | 1.40 | 0.87 |
| 1:A:116:THR:CG2 | 1:A:117:GLU:N | 2.37 | 0.86 |
| 1:A:115:ALA:O | 1:A:116:THR:O | 1.92 | 0.86 |
| 1:A:56:ARG:CD | 1:A:60:GLN:NE2 | 2.38 | 0.86 |
| 2:B:21:ILE:HB | 2:B:22:PRO:HD3 | 1.58 | 0.86 |
| 1:A:145:ILE:C | 1:A:145:ILE:CD1 | 2.38 | 0.86 |
| 2:B:72:ASP:OD1 | 2:B:98:SER:C | 2.13 | 0.86 |
| 2:B:63:ASN:HA | 2:B:84:ASN:HB2 | 1.57 | 0.86 |
| 1:A:145:ILE:O | 1:A:145:ILE:CD1 | 2.22 | 0.86 |
| 1:A:235:VAL:HG23 | 1:A:238:GLN:CA | 2.06 | 0.86 |
| 1:A:197:TYR:CD1 | 1:A:197:TYR:C | 2.44 | 0.86 |
| 1:A:35:GLN:HA | 1:A:35:GLN:HE21 | 1.38 | 0.86 |
| 1:A:303:LEU:CD2 | 1:A:305:LEU:HB3 | 2.05 | 0.86 |
| 2:B:102:ARG:HD2 | 2:B:104:ILE:CD1 | 2.06 | 0.86 |
| 1:A:160:VAL:CG1 | 1:A:187:ILE:HB | 2.03 | 0.86 |
| 1:A:278:ALA:O | 1:A:279:TRP:HB2 | 1.07 | 0.86 |
| 2:B:106:VAL:O | 2:B:107:LEU:HG | 1.76 | 0.86 |
| 2:B:9:VAL:HG21 | 2:B:14:ARG:C | 1.96 | 0.86 |
| 1:A:2:ASN:OD1 | 1:A:2:ASN:C | 2.12 | 0.85 |
| 1:A:40:LYS:O | 1:A:41:HIS:HB2 | 1.74 | 0.85 |
| 2:B:106:VAL:O | 2:B:107:LEU:CB | 2.24 | 0.85 |
| 1:A:198:ILE:O | 1:A:198:ILE:HD12 | 1.75 | 0.85 |
| 1:A:136:THR:HB | 1:A:291:ARG:HH21 | 1.41 | 0.85 |
| 1:A:214:SER:HB3 | 1:A:216:GLU:HB2 | 1.59 | 0.85 |
| 2:B:38:THR:O | 2:B:38:THR:CG2 | 2.24 | 0.85 |
| 1:A:29:LYS:CG | 1:A:30:LEU:N | 2.30 | 0.85 |
| 2:B:101:GLU:O | 2:B:101:GLU:HG3 | 1.76 | 0.85 |
| 1:A:9:ILE:C | 1:A:10:ILE:HD12 | 1.97 | 0.84 |
| 1:A:234:ASX:XD2 | 1:A:234:ASX:H | 1.88 | 0.84 |
| 2:B:18:ILE:HD13 | 2:B:44:ILE:CG1 | 2.07 | 0.84 |
| 2:B:4:ASN:OD1 | 2:B:5:ASP:CA | 2.26 | 0.84 |
| 1:A:91:THR:HG22 | 1:A:95:ILE:HD12 | 1.58 | 0.84 |
| 2:B:67:SER:OG | 2:B:68:GLU:N | 2.10 | 0.84 |
| 1:A:136:THR:HB | 1:A:291:ARG:NH2 | 1.92 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:160:VAL:HG12 | 1:A:187:ILE:CB | 2.03 | 0.83 |
| 1:A:235:VAL:HG22 | 1:A:238:GLN:HB2 | 1.60 | 0.83 |
| 1:A:249:LEU:C | 1:A:250:HIS:ND1 | 2.31 | 0.83 |
| 2:B:128:ARG:HH21 | 2:B:128:ARG:CB | 1.90 | 0.83 |
| 1:A:212:HIS:ND1 | 1:A:212:HIS:N | 2.22 | 0.83 |
| 2:B:114:CYS:SG | 2:B:116:SER:OG | 2.31 | 0.83 |
| 2:B:106:VAL:O | 2:B:107:LEU:CG | 2.27 | 0.83 |
| 1:A:92:ILE:O | 1:A:95:ILE:HG22 | 1.77 | 0.83 |
| 1:A:5:TYR:CE2 | 1:A:300:ASN:O | 2.31 | 0.83 |
| 1:A:95:ILE:HG22 | 1:A:96:SER:H | 1.39 | 0.83 |
| 2:B:106:VAL:O | 2:B:107:LEU:HB2 | 1.78 | 0.83 |
| 2:B:119:GLU:CB | 2:B:120:PRO:CD | 2.55 | 0.83 |
| 1:A:211:LEU:C | 1:A:212:HIS:ND1 | 2.32 | 0.83 |
| 1:A:279:TRP:HA | 1:A:282:GLN:NE2 | 1.94 | 0.83 |
| 2:B:28:LYS:C | 2:B:32:LEU:HB2 | 1.99 | 0.82 |
| 1:A:189:PRO:HG2 | 1:A:189:PRO:O | 1.76 | 0.82 |
| 2:B:66:LEU:H | 2:B:66:LEU:HD13 | 0.66 | 0.82 |
| 1:A:228:ASP:O | 1:A:267:GLU:HG2 | 1.78 | 0.82 |
| 2:B:69:ASP:CG | 2:B:69:ASP:O | 2.16 | 0.82 |
| 1:A:202:LEU:HD12 | 1:A:207:ILE:CG2 | 2.08 | 0.82 |
| 1:A:250:HIS:O | 1:A:252:ALA:N | 2.12 | 0.82 |
| 1:A:260:HIS:H | 1:A:283:GLN:NE2 | 1.78 | 0.82 |
| 2:B:9:VAL:CG2 | 2:B:14:ARG:C | 2.48 | 0.82 |
| 1:A:22:LEU:O | 1:A:26:THR:N | 2.13 | 0.82 |
| 2:B:29:LEU:HD23 | 2:B:33:PHE:HE1 | 1.45 | 0.82 |
| 1:A:262:LEU:CB | 1:A:263:PRO:HA | 2.07 | 0.82 |
| 1:A:162:ASP:HA | 1:A:192:LEU:HB3 | 1.61 | 0.82 |
| 1:A:191:ALA:C | 1:A:192:LEU:HD13 | 2.00 | 0.82 |
| 1:A:201:MET:HA | 1:A:204:GLU:HG3 | 1.62 | 0.82 |
| 2:B:145:SER:O | 2:B:146:HIS:C | 2.18 | 0.82 |
| 2:B:22:PRO:CG | 2:B:25:ILE:HG23 | 2.09 | 0.81 |
| 1:A:228:ASP:CB | 1:A:229:PRO:HD3 | 2.01 | 0.81 |
| 2:B:18:ILE:O | 2:B:43:THR:O | 1.99 | 0.81 |
| 1:A:208:ALA:O | 1:A:209:TRP:CB | 2.27 | 0.81 |
| 1:A:95:ILE:CG2 | 1:A:96:SER:N | 2.42 | 0.81 |
| 1:A:187:ILE:HG21 | 1:A:214:SER:O | 1.80 | 0.81 |
| 1:A:235:VAL:HG23 | 1:A:238:GLN:CB | 2.11 | 0.81 |
| 2:B:18:ILE:HD13 | 2:B:44:ILE:HG12 | 1.63 | 0.81 |
| 2:B:29:LEU:O | 2:B:33:PHE:N | 2.13 | 0.81 |
| 1:A:108:GLN:HG3 | 2:B:113:ASN:ND2 | 1.95 | 0.81 |
| 2:B:17:VAL:HA | 2:B:18:ILE:HD12 | 1.62 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:86:ILE:O | 2:B:90:GLU:OE2 | 1.97 | 0.81 |
| 1:A:208:ALA:HA | 1:A:209:TRP:HD1 | 1.44 | 0.80 |
| 2:B:69:ASP:HB2 | 2:B:72:ASP:HB2 | 1.61 | 0.80 |
| 2:B:74:LEU:N | 2:B:74:LEU:CD1 | 2.43 | 0.80 |
| 1:A:152:LEU:CD2 | 1:A:176:LEU:HD21 | 2.11 | 0.80 |
| 1:A:179:PHE:H | 1:A:179:PHE:HD2 | 1.29 | 0.80 |
| 1:A:35:GLN:HE21 | 1:A:35:GLN:N | 1.79 | 0.80 |
| 2:B:4:ASN:CG | 2:B:5:ASP:N | 2.23 | 0.80 |
| 1:A:211:LEU:C | 1:A:212:HIS:CE1 | 2.55 | 0.80 |
| 1:A:257:LYS:HA | 1:A:277:HIS:CA | 2.08 | 0.80 |
| 1:A:31:LYS:NZ | 1:A:286:ASN:OD1 | 2.13 | 0.79 |
| 1:A:75:ASP:CG | 1:A:79:THR:HB | 2.02 | 0.79 |
| 2:B:83:VAL:HG23 | 2:B:92:VAL:HG11 | 1.61 | 0.79 |
| 2:B:9:VAL:HG13 | 2:B:14:ARG:HA | 0.82 | 0.79 |
| 1:A:279:TRP:O | 1:A:280:TYR:C | 2.19 | 0.79 |
| 2:B:129:ARG:O | 2:B:130:ALA:C | 2.21 | 0.79 |
| 1:A:230:SER:O | 1:A:231:GLU:OE1 | 2.00 | 0.79 |
| 2:B:100:PRO:O | 2:B:101:GLU:CG | 2.30 | 0.79 |
| 2:B:26:GLY:O | 2:B:30:LEU:CD1 | 2.29 | 0.79 |
| 1:A:197:TYR:HD1 | 1:A:197:TYR:C | 1.84 | 0.79 |
| 1:A:217:GLU:HG3 | 1:A:221:ARG:HH12 | 1.47 | 0.79 |
| 1:A:10:ILE:CG2 | 1:A:10:ILE:O | 2.21 | 0.79 |
| 1:A:8:HIS:CB | 1:A:10:ILE:HD11 | 2.12 | 0.79 |
| 1:A:212:HIS:CG | 1:A:218:VAL:HG21 | 2.18 | 0.79 |
| 1:A:29:LYS:O | 1:A:33:ASN:N | 2.15 | 0.79 |
| 1:A:254:MET:O | 1:A:255:ASN:CG | 2.21 | 0.79 |
| 2:B:83:VAL:HG23 | 2:B:92:VAL:CG1 | 2.12 | 0.79 |
| 1:A:211:LEU:HD23 | 1:A:211:LEU:N | 1.89 | 0.78 |
| 1:A:22:LEU:O | 1:A:26:THR:OG1 | 2.01 | 0.78 |
| 2:B:29:LEU:HA | 2:B:32:LEU:HB3 | 1.65 | 0.78 |
| 2:B:102:ARG:HD2 | 2:B:104:ILE:HD11 | 1.63 | 0.78 |
| 2:B:150:LEU:O | 2:B:151:ALA:CB | 2.26 | 0.78 |
| 1:A:58:SER:O | 1:A:59:PHE:O | 2.02 | 0.78 |
| 2:B:61:ILE:CG2 | 2:B:62:GLU:HG2 | 2.12 | 0.78 |
| 1:A:198:ILE:CG1 | 1:A:198:ILE:O | 2.28 | 0.78 |
| 2:B:128:ARG:O | 2:B:134:ALA:CB | 2.32 | 0.78 |
| 1:A:66:LEU:CD1 | 1:A:292:GLN:HG3 | 2.14 | 0.78 |
| 2:B:16:THR:HG23 | 2:B:62:GLU:HB3 | 1.66 | 0.78 |
| 1:A:155:LEU:O | 1:A:182:ASN:O | 2.02 | 0.78 |
| 2:B:116:SER:O | 2:B:117:HIS:CB | 2.29 | 0.78 |
| 1:A:132:ASN:HD21 | 2:B:141:GLU:HB2 | 1.46 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:47:ASN:C | 2:B:49:PRO:N | 2.30 | 0.78 |
| 1:A:214:SER:HB3 | 1:A:216:GLU:CG | 2.14 | 0.78 |
| 1:A:274:LYS:HD2 | 1:A:275:THR:CA | 2.14 | 0.78 |
| 2:B:115:ILE:CG2 | 2:B:119:GLU:HG3 | 2.14 | 0.78 |
| 2:B:147:ASN:O | 2:B:148:VAL:C | 2.22 | 0.78 |
| 2:B:28:LYS:O | 2:B:32:LEU:HB2 | 1.82 | 0.78 |
| 2:B:61:ILE:HG23 | 2:B:62:GLU:CG | 2.11 | 0.78 |
| 1:A:251:ASN:O | 1:A:253:LYS:HG3 | 1.83 | 0.78 |
| 2:B:18:ILE:CD1 | 2:B:18:ILE:N | 2.45 | 0.77 |
| 1:A:208:ALA:C | 1:A:209:TRP:CD1 | 2.58 | 0.77 |
| 1:A:207:ILE:HG23 | 1:A:208:ALA:N | 1.98 | 0.77 |
| 1:A:303:LEU:HD11 | 1:A:305:LEU:CB | 2.13 | 0.77 |
| 2:B:77:TYR:N | 2:B:77:TYR:CD1 | 2.51 | 0.77 |
| 1:A:81:LEU:CD2 | 1:A:82:GLY:H | 1.96 | 0.77 |
| 1:A:82:GLY:HA3 | 1:A:86:GLN:HB3 | 1.66 | 0.77 |
| 2:B:26:GLY:O | 2:B:30:LEU:HD12 | 1.84 | 0.77 |
| 2:B:61:ILE:CB | 2:B:82:THR:O | 2.30 | 0.77 |
| 1:A:109:GLU:HA | 1:A:129:ASP:HB3 | 1.65 | 0.77 |
| 1:A:119:SER:OG | 1:A:119:SER:O | 1.94 | 0.77 |
| 1:A:210:SER:O | 1:A:211:LEU:CD2 | 2.29 | 0.77 |
| 2:B:17:VAL:CG1 | 2:B:43:THR:HB | 2.15 | 0.77 |
| 2:B:115:ILE:HG22 | 2:B:119:GLU:HG3 | 1.66 | 0.77 |
| 2:B:137:CYS:SG | 2:B:139:TYR:HB2 | 2.24 | 0.77 |
| 1:A:136:THR:CG2 | 1:A:291:ARG:NH2 | 2.48 | 0.77 |
| 1:A:141:ASP:O | 1:A:145:ILE:HG22 | 1.85 | 0.77 |
| 2:B:86:ILE:O | 2:B:90:GLU:HG3 | 1.84 | 0.77 |
| 2:B:27:PHE:O | 2:B:30:LEU:CB | 2.32 | 0.76 |
| 1:A:136:THR:CB | 1:A:291:ARG:HH21 | 1.98 | 0.76 |
| 1:A:39:LEU:O | 1:A:42:LYS:HB2 | 1.84 | 0.76 |
| 2:B:34:LYS:C | 2:B:35:LEU:HG | 2.03 | 0.76 |
| 1:A:294:LEU:O | 1:A:298:VAL:CG2 | 2.21 | 0.76 |
| 1:A:75:ASP:OD1 | 1:A:79:THR:HB | 1.84 | 0.76 |
| 2:B:30:LEU:O | 2:B:33:PHE:O | 2.02 | 0.76 |
| 2:B:72:ASP:CG | 2:B:98:SER:O | 2.24 | 0.76 |
| 2:B:5:ASP:OD1 | 2:B:6:LYS:N | 2.17 | 0.76 |
| 1:A:164:LYS:HD3 | 1:A:165:TYR:HE2 | 1.49 | 0.76 |
| 1:A:9:ILE:HD13 | 1:A:294:LEU:HD22 | 1.67 | 0.76 |
| 1:A:111:ALA:O | 1:A:112:ALA:C | 2.22 | 0.76 |
| 1:A:16:SER:HB3 | 1:A:19:ASP:OD1 | 1.85 | 0.76 |
| 1:A:87:THR:C | 1:A:89:ALA:H | 1.90 | 0.76 |
| 2:B:71:VAL:C | 2:B:73:GLU:N | 2.28 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:18:ILE:HD12 | 2:B:18:ILE:N | 1.99 | 0.76 |
| 1:A:194:MET:HG3 | 1:A:195:PRO:HD2 | 1.68 | 0.75 |
| 1:A:194:MET:CE | 1:A:198:ILE:HG13 | 2.16 | 0.75 |
| 1:A:52:SER:OG | 1:A:55:THR:HG21 | 1.85 | 0.75 |
| 2:B:67:SER:CB | 2:B:70:GLU:OE2 | 2.33 | 0.75 |
| 1:A:214:SER:HB3 | 1:A:216:GLU:CB | 2.15 | 0.75 |
| 1:A:234:ASX:XD1 | 1:A:239:PHE:CE1 | 2.69 | 0.75 |
| 1:A:152:LEU:HD22 | 1:A:176:LEU:CD2 | 2.15 | 0.75 |
| 1:A:177:ALA:O | 1:A:178:LYS:C | 2.23 | 0.75 |
| 1:A:198:ILE:O | 1:A:198:ILE:CD1 | 2.34 | 0.75 |
| 1:A:110:GLY:O | 1:A:113:ARG:N | 2.20 | 0.75 |
| 1:A:140:LEU:CD1 | 1:A:287:GLY:CA | 2.59 | 0.75 |
| 1:A:303:LEU:HG | 1:A:305:LEU:H | 1.51 | 0.75 |
| 2:B:28:LYS:O | 2:B:31:SER:OG | 2.04 | 0.75 |
| 1:A:93:SER:C | 1:A:96:SER:OG | 2.25 | 0.75 |
| 2:B:16:THR:O | 2:B:17:VAL:CG2 | 2.33 | 0.75 |
| 2:B:1:MET:HE1 | 2:B:41:ARG:HH22 | 1.51 | 0.75 |
| 1:A:179:PHE:HD2 | 1:A:179:PHE:N | 1.85 | 0.75 |
| 1:A:194:MET:HE2 | 1:A:198:ILE:HG13 | 1.67 | 0.75 |
| 1:A:159:MET:HE1 | 1:A:172:LEU:CD2 | 2.17 | 0.74 |
| 2:B:60:LYS:O | 2:B:82:THR:O | 2.04 | 0.74 |
| 1:A:116:THR:HG22 | 1:A:117:GLU:H | 1.52 | 0.74 |
| 1:A:266:ASP:O | 1:A:267:GLU:C | 2.18 | 0.74 |
| 1:A:87:THR:C | 1:A:89:ALA:N | 2.39 | 0.74 |
| 2:B:146:HIS:O | 2:B:150:LEU:HB2 | 1.87 | 0.74 |
| 2:B:5:ASP:CG | 2:B:6:LYS:N | 2.40 | 0.74 |
| 1:A:195:PRO:O | 1:A:199:LEU:HD13 | 1.88 | 0.74 |
| 1:A:230:SER:H | 1:A:231:GLU:HG2 | 1.50 | 0.74 |
| 2:B:72:ASP:OD1 | 2:B:98:SER:O | 2.05 | 0.74 |
| 2:B:137:CYS:O | 2:B:137:CYS:SG | 2.45 | 0.74 |
| 1:A:45:ALA:HB2 | 1:A:99:VAL:HG11 | 1.68 | 0.74 |
| 1:A:132:ASN:ND2 | 2:B:141:GLU:HB2 | 2.02 | 0.74 |
| 1:A:253:LYS:C | 1:A:254:MET:HG2 | 2.08 | 0.74 |
| 2:B:16:THR:CG2 | 2:B:62:GLU:HB3 | 2.18 | 0.74 |
| 1:A:232:TYR:O | 1:A:234:ASX:CG | 2.26 | 0.73 |
| 1:A:246:LEU:O | 1:A:268:ILE:HA | 1.88 | 0.73 |
| 1:A:29:LYS:N | 1:A:29:LYS:HD2 | 2.02 | 0.73 |
| 2:B:18:ILE:HD12 | 2:B:43:THR:O | 1.87 | 0.73 |
| 1:A:175:ALA:O | 1:A:177:ALA:N | 2.22 | 0.73 |
| 1:A:80:SER:O | 1:A:81:LEU:CD1 | 2.35 | 0.73 |
| 1:A:294:LEU:O | 1:A:298:VAL:N | 2.20 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:41:HIS:N | 1:A:41:HIS:CD2 | 2.53 | 0.73 |
| 1:A:115:ALA:O | 1:A:116:THR:C | 2.19 | 0.73 |
| 2:B:147:ASN:O | 2:B:149:VAL:HB | 1.89 | 0.73 |
| 2:B:32:LEU:CD2 | 2:B:77:TYR:CE2 | 2.65 | 0.73 |
| 1:A:59:PHE:O | 1:A:62:SER:CB | 2.31 | 0.73 |
| 1:A:199:LEU:C | 1:A:201:MET:N | 2.36 | 0.73 |
| 1:A:42:LYS:O | 1:A:69:SER:OG | 2.02 | 0.73 |
| 1:A:81:LEU:HD13 | 1:A:82:GLY:O | 1.89 | 0.73 |
| 1:A:232:TYR:CD2 | 1:A:232:TYR:N | 2.57 | 0.73 |
| 2:B:61:ILE:HG22 | 2:B:62:GLU:CA | 2.19 | 0.72 |
| 1:A:259:LEU:CD1 | 1:A:259:LEU:N | 2.52 | 0.72 |
| 1:A:80:SER:O | 1:A:81:LEU:HB3 | 1.88 | 0.72 |
| 1:A:198:ILE:C | 1:A:198:ILE:HD12 | 2.10 | 0.72 |
| 1:A:257:LYS:CA | 1:A:277:HIS:HA | 2.10 | 0.72 |
| 1:A:303:LEU:HD21 | 1:A:305:LEU:HD22 | 1.71 | 0.72 |
| 1:A:95:ILE:O | 1:A:99:VAL:HG22 | 1.89 | 0.72 |
| 1:A:240:LEU:HD22 | 1:A:241:VAL:HG22 | 1.72 | 0.72 |
| 2:B:25:ILE:HD12 | 2:B:25:ILE:C | 2.09 | 0.72 |
| 2:B:74:LEU:O | 2:B:76:LEU:N | 2.22 | 0.72 |
| 1:A:29:LYS:C | 1:A:31:LYS:N | 2.40 | 0.72 |
| 1:A:251:ASN:C | 1:A:253:LYS:N | 2.34 | 0.72 |
| 1:A:17:ARG:O | 1:A:19:ASP:N | 2.23 | 0.72 |
| 1:A:274:LYS:HD2 | 1:A:275:THR:HA | 1.72 | 0.72 |
| 1:A:56:ARG:NE | 1:A:60:GLN:HE22 | 1.86 | 0.72 |
| 2:B:9:VAL:CG1 | 2:B:10:ALA:H | 2.02 | 0.72 |
| 1:A:148:THR:OG1 | 1:A:149:GLU:HG2 | 1.89 | 0.72 |
| 1:A:184:PHE:CE1 | 1:A:202:LEU:HD11 | 2.25 | 0.72 |
| 1:A:17:ARG:O | 1:A:18:ASP:C | 2.27 | 0.72 |
| 2:B:71:VAL:O | 2:B:73:GLU:CB | 2.38 | 0.72 |
| 2:B:64:THR:N | 2:B:84:ASN:ND2 | 2.38 | 0.72 |
| 2:B:18:ILE:O | 2:B:44:ILE:HG12 | 1.89 | 0.72 |
| 2:B:16:THR:HA | 2:B:64:THR:OG1 | 1.90 | 0.72 |
| 2:B:79:PRO:HG2 | 2:B:80:GLN:N | 2.05 | 0.72 |
| 1:A:303:LEU:HG | 1:A:304:VAL:N | 2.05 | 0.71 |
| 1:A:274:LYS:HD2 | 1:A:275:THR:N | 2.05 | 0.71 |
| 2:B:145:SER:C | 2:B:147:ASN:N | 2.44 | 0.71 |
| 2:B:29:LEU:CD2 | 2:B:33:PHE:HE1 | 2.03 | 0.71 |
| 2:B:61:ILE:HG22 | 2:B:62:GLU:O | 1.91 | 0.71 |
| 1:A:119:SER:C | 1:A:120:GLY:O | 2.25 | 0.71 |
| 1:A:18:ASP:O | 1:A:19:ASP:C | 2.28 | 0.71 |
| 2:B:36:THR:CG2 | 2:B:36:THR:O | 2.38 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:175:ALA:O | 1:A:176:LEU:C | 2.24 | 0.71 |
| 2:B:1:MET:HE3 | 2:B:41:ARG:HH22 | 1.56 | 0.71 |
| 2:B:77:TYR:N | 2:B:77:TYR:HD1 | 1.88 | 0.71 |
| 1:A:35:GLN:HA | 1:A:35:GLN:NE2 | 2.02 | 0.70 |
| 1:A:208:ALA:C | 1:A:209:TRP:HD1 | 1.94 | 0.70 |
| 2:B:29:LEU:HD23 | 2:B:33:PHE:CE1 | 2.26 | 0.70 |
| 2:B:46:LEU:O | 2:B:46:LEU:HD23 | 1.91 | 0.70 |
| 1:A:273:ASP:HA | 1:A:280:TYR:OH | 1.92 | 0.70 |
| 1:A:293:ALA:O | 1:A:297:LEU:CD1 | 2.39 | 0.70 |
| 1:A:35:GLN:HB3 | 1:A:38:LEU:CD2 | 2.20 | 0.70 |
| 2:B:62:GLU:C | 2:B:63:ASN:OD1 | 2.29 | 0.70 |
| 2:B:69:ASP:OD1 | 2:B:69:ASP:O | 2.09 | 0.70 |
| 1:A:136:THR:CB | 1:A:291:ARG:NH2 | 2.54 | 0.70 |
| 1:A:138:THR:HG21 | 1:A:171:SER:HB2 | 1.72 | 0.70 |
| 1:A:276:PRO:C | 1:A:278:ALA:H | 1.95 | 0.70 |
| 1:A:137:GLN:O | 1:A:140:LEU:HB3 | 1.92 | 0.70 |
| 1:A:161:GLY:HA3 | 1:A:228:ASP:CG | 2.11 | 0.70 |
| 2:B:18:ILE:CD1 | 2:B:44:ILE:HG12 | 2.20 | 0.70 |
| 1:A:214:SER:CB | 1:A:216:GLU:HG3 | 2.20 | 0.70 |
| 1:A:251:ASN:O | 1:A:253:LYS:CB | 2.40 | 0.70 |
| 1:A:230:SER:O | 1:A:231:GLU:CG | 2.40 | 0.70 |
| 1:A:249:LEU:O | 1:A:250:HIS:CG | 2.43 | 0.70 |
| 2:B:114:CYS:HG | 2:B:140:CYS:HG | 1.38 | 0.70 |
| 1:A:114:LEU:HD23 | 1:A:114:LEU:C | 2.12 | 0.70 |
| 1:A:260:HIS:O | 1:A:262:LEU:N | 2.23 | 0.70 |
| 1:A:38:LEU:HB3 | 1:A:39:LEU:HD23 | 1.74 | 0.70 |
| 1:A:157:VAL:HG12 | 1:A:183:ARG:O | 1.92 | 0.69 |
| 1:A:76:SER:O | 1:A:77:ALA:CB | 2.38 | 0.69 |
| 2:B:134:ALA:O | 2:B:135:LEU:HD12 | 1.91 | 0.69 |
| 2:B:98:SER:O | 2:B:99:LEU:O | 2.10 | 0.69 |
| 1:A:272:VAL:C | 1:A:273:ASP:O | 2.29 | 0.69 |
| 2:B:108:VAL:CG2 | 2:B:152:ASN:HB3 | 2.21 | 0.69 |
| 1:A:35:GLN:CG | 1:A:38:LEU:HD21 | 2.19 | 0.69 |
| 1:A:304:VAL:HG23 | 1:A:304:VAL:O | 1.92 | 0.69 |
| 2:B:107:LEU:HB3 | 2:B:125:PHE:CE1 | 2.26 | 0.69 |
| 2:B:75:ALA:HB1 | 2:B:99:LEU:HD22 | 1.74 | 0.69 |
| 1:A:81:LEU:HD22 | 1:A:82:GLY:O | 1.92 | 0.69 |
| 1:A:88:LEU:CD2 | 1:A:88:LEU:O | 2.41 | 0.69 |
| 1:A:297:LEU:O | 1:A:298:VAL:C | 2.30 | 0.69 |
| 2:B:17:VAL:HG22 | 2:B:43:THR:OG1 | 1.92 | 0.69 |
| 2:B:86:ILE:CG2 | 2:B:90:GLU:HB2 | 2.20 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:140:LEU:CD1 | 1:A:287:GLY:HA2 | 2.13 | 0.69 |
| 1:A:60:GLN:O | 1:A:63:MET:N | 2.26 | 0.69 |
| 1:A:83:LYS:O | 1:A:84:LYS:C | 2.31 | 0.69 |
| 1:A:211:LEU:O | 1:A:212:HIS:CD2 | 2.46 | 0.69 |
| 1:A:141:ASP:HA | 1:A:144:THR:HG21 | 1.75 | 0.69 |
| 2:B:111:ASP:HB2 | 2:B:144:PHE:HZ | 1.58 | 0.69 |
| 2:B:68:GLU:O | 2:B:70:GLU:N | 2.25 | 0.69 |
| 2:B:124:SER:HB3 | 2:B:138:LYS:HE3 | 1.73 | 0.68 |
| 2:B:46:LEU:HD21 | 2:B:48:LEU:HG | 1.75 | 0.68 |
| 1:A:158:ALA:HA | 1:A:185:TYR:HB2 | 1.74 | 0.68 |
| 2:B:92:VAL:HG12 | 2:B:92:VAL:O | 1.92 | 0.68 |
| 1:A:219:MET:O | 1:A:219:MET:CG | 2.24 | 0.68 |
| 2:B:15:GLY:O | 2:B:64:THR:CB | 2.40 | 0.68 |
| 1:A:163:LEU:HD22 | 1:A:188:ALA:HB2 | 1.76 | 0.68 |
| 1:A:88:LEU:C | 1:A:88:LEU:CD2 | 2.62 | 0.68 |
| 1:A:68:ALA:C | 1:A:69:SER:OG | 2.28 | 0.68 |
| 2:B:11:GLU:O | 2:B:12:ILE:C | 2.30 | 0.68 |
| 2:B:72:ASP:O | 2:B:100:PRO:HG3 | 1.92 | 0.68 |
| 2:B:76:LEU:HB3 | 2:B:77:TYR:CD1 | 2.28 | 0.68 |
| 1:A:184:PHE:CD1 | 1:A:202:LEU:HD11 | 2.29 | 0.68 |
| 1:A:77:ALA:C | 1:A:79:THR:H | 1.97 | 0.68 |
| 2:B:107:LEU:HD21 | 2:B:150:LEU:HD22 | 1.75 | 0.68 |
| 1:A:280:TYR:O | 1:A:283:GLN:HB3 | 1.92 | 0.67 |
| 2:B:106:VAL:HG13 | 2:B:106:VAL:O | 1.95 | 0.67 |
| 2:B:39:GLN:NE2 | 2:B:40:ASP:H | 1.92 | 0.67 |
| 1:A:215:ILE:HG21 | 1:A:246:LEU:HD23 | 1.76 | 0.67 |
| 1:A:276:PRO:C | 1:A:278:ALA:N | 2.48 | 0.67 |
| 1:A:71:VAL:HG23 | 1:A:71:VAL:O | 1.93 | 0.67 |
| 2:B:111:ASP:O | 2:B:117:HIS:CE1 | 2.43 | 0.67 |
| 1:A:179:PHE:CD2 | 1:A:179:PHE:N | 2.62 | 0.67 |
| 1:A:274:LYS:CD | 1:A:275:THR:CA | 2.72 | 0.67 |
| 1:A:272:VAL:O | 1:A:275:THR:HG23 | 1.95 | 0.67 |
| 1:A:44:ILE:HG22 | 1:A:45:ALA:H | 1.59 | 0.67 |
| 1:A:209:TRP:N | 1:A:209:TRP:CD1 | 2.61 | 0.67 |
| 2:B:81:ALA:O | 2:B:82:THR:HG23 | 1.95 | 0.67 |
| 2:B:25:ILE:C | 2:B:25:ILE:CD1 | 2.62 | 0.67 |
| 2:B:20:HIS:CE1 | 2:B:47:ASN:HB2 | 2.30 | 0.67 |
| 1:A:113:ARG:O | 1:A:116:THR:N | 2.28 | 0.66 |
| 1:A:114:LEU:O | 1:A:114:LEU:HD23 | 1.95 | 0.66 |
| 1:A:162:ASP:O | 1:A:162:ASP:OD1 | 2.13 | 0.66 |
| 1:A:231:GLU:O | 1:A:232:TYR:O | 2.11 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:2:ASN:OD1 | 1:A:4:LEU:N | 2.28 | 0.66 |
| 2:B:18:ILE:CG2 | 2:B:62:GLU:OE2 | 2.31 | 0.66 |
| 2:B:5:ASP:OD1 | 2:B:5:ASP:C | 2.32 | 0.66 |
| 1:A:10:ILE:O | 1:A:11:SER:CB | 2.42 | 0.66 |
| 2:B:12:ILE:O | 2:B:13:LYS:CG | 2.43 | 0.66 |
| 2:B:27:PHE:C | 2:B:30:LEU:HD12 | 2.15 | 0.66 |
| 1:A:303:LEU:HD11 | 1:A:305:LEU:HB2 | 1.77 | 0.66 |
| 1:A:35:GLN:HB3 | 1:A:38:LEU:HD23 | 1.78 | 0.66 |
| 1:A:49:PHE:CE1 | 1:A:104:MET:HE2 | 2.30 | 0.66 |
| 1:A:231:GLU:CB | 1:A:232:TYR:HE2 | 2.03 | 0.66 |
| 1:A:34:PRO:O | 1:A:35:GLN:NE2 | 2.28 | 0.66 |
| 1:A:189:PRO:CG | 1:A:189:PRO:O | 2.36 | 0.66 |
| 1:A:11:SER:HA | 1:A:133:GLN:HG2 | 1.78 | 0.66 |
| 1:A:303:LEU:C | 1:A:303:LEU:HD23 | 2.16 | 0.66 |
| 1:A:136:THR:HG21 | 1:A:291:ARG:NE | 2.10 | 0.65 |
| 1:A:70:VAL:O | 1:A:71:VAL:CG1 | 2.38 | 0.65 |
| 2:B:4:ASN:OD1 | 2:B:5:ASP:C | 2.34 | 0.65 |
| 1:A:44:ILE:O | 1:A:71:VAL:HG21 | 1.94 | 0.65 |
| 1:A:135:PRO:O | 1:A:139:LEU:HG | 1.95 | 0.65 |
| 1:A:249:LEU:O | 1:A:250:HIS:CE1 | 2.49 | 0.65 |
| 2:B:39:GLN:CG | 2:B:40:ASP:H | 2.10 | 0.65 |
| 1:A:80:SER:O | 1:A:81:LEU:CB | 2.44 | 0.65 |
| 1:A:38:LEU:C | 1:A:39:LEU:HD23 | 2.17 | 0.65 |
| 2:B:10:ALA:O | 2:B:11:GLU:CB | 2.44 | 0.65 |
| 1:A:279:TRP:C | 1:A:281:PHE:N | 2.44 | 0.65 |
| 2:B:116:SER:HA | 2:B:121:VAL:HG11 | 1.79 | 0.65 |
| 2:B:60:LYS:O | 2:B:61:ILE:CB | 2.45 | 0.65 |
| 1:A:201:MET:HA | 1:A:204:GLU:CG | 2.26 | 0.65 |
| 1:A:230:SER:N | 1:A:231:GLU:HG2 | 2.11 | 0.65 |
| 1:A:231:GLU:HB3 | 1:A:232:TYR:CD2 | 2.32 | 0.65 |
| 1:A:40:LYS:CB | 1:A:41:HIS:CD2 | 2.79 | 0.65 |
| 2:B:71:VAL:O | 2:B:73:GLU:CA | 2.44 | 0.65 |
| 2:B:28:LYS:HB3 | 2:B:32:LEU:HD12 | 1.79 | 0.65 |
| 2:B:69:ASP:HA | 2:B:71:VAL:HB | 1.77 | 0.65 |
| 1:A:49:PHE:CE1 | 1:A:104:MET:CE | 2.79 | 0.64 |
| 1:A:18:ASP:O | 1:A:21:ASN:N | 2.30 | 0.64 |
| 2:B:148:VAL:HG13 | 2:B:148:VAL:O | 1.96 | 0.64 |
| 2:B:17:VAL:CA | 2:B:18:ILE:HD12 | 2.27 | 0.64 |
| 2:B:18:ILE:HG23 | 2:B:62:GLU:CD | 2.17 | 0.64 |
| 2:B:86:ILE:N | 2:B:90:GLU:HB2 | 2.12 | 0.64 |
| 1:A:274:LYS:O | 1:A:274:LYS:HD3 | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:2:ASN:OD1 | 1:A:3:PRO:N | 2.30 | 0.64 |
| 2:B:102:ARG:O | 2:B:104:ILE:HD12 | 1.96 | 0.64 |
| 2:B:116:SER:O | 2:B:117:HIS:CG | 2.49 | 0.64 |
| 2:B:17:VAL:HG22 | 2:B:43:THR:HB | 1.79 | 0.64 |
| 2:B:39:GLN:HG2 | 2:B:40:ASP:N | 2.12 | 0.64 |
| 2:B:4:ASN:O | 2:B:43:THR:HG21 | 1.96 | 0.64 |
| 1:A:82:GLY:HA3 | 1:A:86:GLN:CB | 2.27 | 0.64 |
| 1:A:9:ILE:HB | 1:A:125:LEU:HD12 | 1.78 | 0.64 |
| 1:A:49:PHE:CD1 | 1:A:104:MET:HE2 | 2.32 | 0.64 |
| 2:B:31:SER:C | 2:B:33:PHE:N | 2.45 | 0.64 |
| 1:A:230:SER:O | 1:A:231:GLU:HG2 | 1.98 | 0.64 |
| 1:A:77:ALA:O | 1:A:79:THR:N | 2.30 | 0.64 |
| 2:B:147:ASN:O | 2:B:148:VAL:O | 2.16 | 0.64 |
| 2:B:17:VAL:HA | 2:B:18:ILE:CD1 | 2.28 | 0.64 |
| 2:B:64:THR:H | 2:B:84:ASN:HD22 | 1.44 | 0.64 |
| 1:A:204:GLU:OE2 | 1:A:205:LYS:NZ | 2.31 | 0.64 |
| 1:A:40:LYS:O | 1:A:41:HIS:CB | 2.44 | 0.64 |
| 1:A:251:ASN:O | 1:A:253:LYS:CG | 2.46 | 0.64 |
| 1:A:9:ILE:HD13 | 1:A:294:LEU:CD2 | 2.28 | 0.64 |
| 2:B:86:ILE:O | 2:B:90:GLU:CD | 2.36 | 0.64 |
| 1:A:101:ALA:C | 1:A:102:ILE:HG12 | 2.18 | 0.64 |
| 1:A:275:THR:O | 1:A:276:PRO:O | 2.15 | 0.64 |
| 1:A:34:PRO:C | 1:A:35:GLN:HE21 | 2.01 | 0.64 |
| 1:A:212:HIS:CG | 1:A:218:VAL:CG2 | 2.82 | 0.63 |
| 1:A:58:SER:O | 1:A:59:PHE:C | 2.37 | 0.63 |
| 2:B:66:LEU:HB2 | 2:B:70:GLU:HB2 | 1.80 | 0.63 |
| 2:B:84:ASN:O | 2:B:92:VAL:HB | 1.99 | 0.63 |
| 1:A:175:ALA:HA | 1:A:178:LYS:HD2 | 1.80 | 0.63 |
| 2:B:20:HIS:CG | 2:B:20:HIS:O | 2.51 | 0.63 |
| 1:A:231:GLU:O | 1:A:234:ASX:XD2 | 2.46 | 0.63 |
| 1:A:140:LEU:CD1 | 1:A:287:GLY:N | 2.61 | 0.63 |
| 1:A:196:GLU:O | 1:A:200:ASP:OD2 | 2.16 | 0.63 |
| 1:A:253:LYS:HD3 | 1:A:277:HIS:NE2 | 2.14 | 0.63 |
| 2:B:18:ILE:HB | 2:B:44:ILE:CD1 | 2.29 | 0.63 |
| 1:A:140:LEU:HD13 | 1:A:287:GLY:N | 2.11 | 0.63 |
| 1:A:159:MET:CE | 1:A:172:LEU:CD2 | 2.75 | 0.63 |
| 2:B:146:HIS:CD2 | 2:B:147:ASN:OD1 | 2.52 | 0.63 |
| 1:A:129:ASP:OD1 | 1:A:132:ASN:OD1 | 2.17 | 0.63 |
| 1:A:81:LEU:CD1 | 1:A:82:GLY:O | 2.47 | 0.63 |
| 1:A:81:LEU:CD2 | 1:A:82:GLY:O | 2.47 | 0.63 |
| 1:A:200:ASP:O | 1:A:204:GLU:N | 2.30 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:39:LEU:O | 1:A:40:LYS:C | 2.37 | 0.62 |
| 2:B:102:ARG:HD2 | 2:B:104:ILE:HD12 | 1.80 | 0.62 |
| 1:A:175:ALA:C | 1:A:177:ALA:N | 2.48 | 0.62 |
| 1:A:218:VAL:O | 1:A:222:VAL:CG2 | 2.47 | 0.62 |
| 1:A:230:SER:C | 1:A:231:GLU:CG | 2.63 | 0.62 |
| 1:A:258:VAL:C | 1:A:259:LEU:CD1 | 2.68 | 0.62 |
| 2:B:146:HIS:CD2 | 2:B:147:ASN:N | 2.68 | 0.62 |
| 2:B:18:ILE:N | 2:B:62:GLU:OE1 | 2.32 | 0.62 |
| 1:A:189:PRO:O | 1:A:191:ALA:N | 2.31 | 0.62 |
| 1:A:274:LYS:CD | 1:A:275:THR:HA | 2.29 | 0.62 |
| 1:A:136:THR:HG21 | 1:A:291:ARG:CD | 2.28 | 0.62 |
| 1:A:201:MET:CG | 1:A:204:GLU:HG3 | 2.29 | 0.62 |
| 1:A:211:LEU:O | 1:A:212:HIS:CE1 | 2.52 | 0.62 |
| 1:A:264:ARG:HG3 | 1:A:265:VAL:N | 2.13 | 0.62 |
| 1:A:8:HIS:H | 1:A:8:HIS:CD2 | 2.18 | 0.62 |
| 2:B:4:ASN:C | 2:B:4:ASN:OD1 | 2.36 | 0.62 |
| 2:B:72:ASP:O | 2:B:75:ALA:CB | 2.46 | 0.62 |
| 1:A:149:GLU:OE2 | 1:A:149:GLU:HA | 2.00 | 0.62 |
| 2:B:146:HIS:CD2 | 2:B:147:ASN:H | 2.16 | 0.62 |
| 2:B:3:HIS:O | 2:B:4:ASN:HB3 | 2.00 | 0.62 |
| 1:A:249:LEU:C | 1:A:250:HIS:CG | 2.69 | 0.62 |
| 1:A:292:GLN:O | 1:A:293:ALA:C | 2.35 | 0.62 |
| 1:A:303:LEU:O | 1:A:303:LEU:CD2 | 2.46 | 0.62 |
| 1:A:81:LEU:HD22 | 1:A:82:GLY:CA | 2.30 | 0.62 |
| 2:B:39:GLN:CG | 2:B:40:ASP:N | 2.62 | 0.62 |
| 1:A:197:TYR:CE1 | 1:A:198:ILE:N | 2.67 | 0.61 |
| 1:A:200:ASP:O | 1:A:204:GLU:HB3 | 2.00 | 0.61 |
| 1:A:221:ARG:O | 1:A:222:VAL:HG23 | 2.00 | 0.61 |
| 1:A:114:LEU:HD13 | 2:B:119:GLU:HG3 | 1.80 | 0.61 |
| 1:A:258:VAL:N | 1:A:277:HIS:O | 2.30 | 0.61 |
| 1:A:40:LYS:HD3 | 1:A:41:HIS:CD2 | 2.33 | 0.61 |
| 2:B:86:ILE:H | 2:B:90:GLU:HG3 | 1.66 | 0.61 |
| 1:A:162:ASP:OD1 | 1:A:162:ASP:C | 2.37 | 0.61 |
| 2:B:12:ILE:O | 2:B:13:LYS:CB | 2.48 | 0.61 |
| 2:B:60:LYS:O | 2:B:61:ILE:HB | 1.99 | 0.61 |
| 2:B:72:ASP:C | 2:B:100:PRO:HG3 | 2.19 | 0.61 |
| 2:B:84:ASN:HB3 | 2:B:92:VAL:HG21 | 1.82 | 0.61 |
| 2:B:15:GLY:O | 2:B:64:THR:OG1 | 2.17 | 0.61 |
| 2:B:79:PRO:O | 2:B:97:PRO:HG2 | 2.01 | 0.61 |
| 1:A:259:LEU:N | 1:A:259:LEU:HD13 | 2.15 | 0.61 |
| 1:A:276:PRO:O | 1:A:277:HIS:C | 2.36 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:61:THR:HG21 | 1:A:288:ILE:HG21 | 1.82 | 0.61 |
| 1:A:111:ALA:O | 1:A:115:ALA:N | 2.33 | 0.61 |
| 1:A:184:PHE:CE1 | 1:A:202:LEU:CD1 | 2.82 | 0.61 |
| 1:A:251:ASN:O | 1:A:252:ALA:C | 2.35 | 0.61 |
| 2:B:133:ILE:HB | 2:B:146:HIS:ND1 | 2.15 | 0.61 |
| 2:B:39:GLN:HG2 | 2:B:40:ASP:H | 1.65 | 0.61 |
| 2:B:1:MET:HE1 | 2:B:41:ARG:NH2 | 2.16 | 0.61 |
| 1:A:262:LEU:HB3 | 1:A:263:PRO:CA | 2.26 | 0.61 |
| 1:A:274:LYS:HB3 | 1:A:275:THR:HG22 | 1.83 | 0.61 |
| 2:B:20:HIS:HB3 | 2:B:46:LEU:HA | 1.81 | 0.61 |
| 1:A:233:ALA:HB3 | 1:A:234:ASX:XD2 | 2.31 | 0.61 |
| 1:A:235:VAL:CG2 | 1:A:238:GLN:CB | 2.72 | 0.61 |
| 1:A:224:LYS:NZ | 1:A:259:LEU:HD11 | 2.15 | 0.61 |
| 1:A:45:ALA:HB2 | 1:A:99:VAL:CG1 | 2.30 | 0.61 |
| 2:B:115:ILE:CG2 | 2:B:119:GLU:CG | 2.78 | 0.61 |
| 2:B:105:ASP:O | 2:B:105:ASP:OD2 | 2.19 | 0.61 |
| 1:A:12:ILE:HG22 | 1:A:13:ASN:N | 2.16 | 0.60 |
| 1:A:141:ASP:C | 1:A:144:THR:CG2 | 2.69 | 0.60 |
| 1:A:138:THR:O | 1:A:142:LEU:HB2 | 2.01 | 0.60 |
| 1:A:143:PHE:O | 1:A:144:THR:C | 2.37 | 0.60 |
| 1:A:161:GLY:HA3 | 1:A:228:ASP:OD1 | 2.00 | 0.60 |
| 1:A:50:GLU:O | 1:A:51:ALA:C | 2.40 | 0.60 |
| 1:A:66:LEU:HD12 | 1:A:292:GLN:HG3 | 1.82 | 0.60 |
| 1:A:16:SER:CB | 1:A:19:ASP:OD1 | 2.48 | 0.60 |
| 1:A:16:SER:OG | 1:A:18:ASP:HB2 | 2.00 | 0.60 |
| 1:A:281:PHE:O | 1:A:283:GLN:N | 2.35 | 0.60 |
| 2:B:23:ALA:O | 2:B:24:GLU:HB3 | 1.99 | 0.60 |
| 1:A:163:LEU:HB2 | 1:A:192:LEU:O | 2.02 | 0.60 |
| 1:A:187:ILE:HA | 1:A:212:HIS:O | 2.00 | 0.60 |
| 1:A:20:LEU:O | 1:A:24:LEU:CD2 | 2.49 | 0.60 |
| 1:A:266:ASP:O | 1:A:268:ILE:N | 2.35 | 0.60 |
| 1:A:304:VAL:CG2 | 1:A:304:VAL:O | 2.49 | 0.60 |
| 2:B:100:PRO:C | 2:B:101:GLU:HG2 | 2.21 | 0.60 |
| 2:B:17:VAL:CG2 | 2:B:43:THR:CB | 2.77 | 0.60 |
| 2:B:63:ASN:HB3 | 2:B:84:ASN:HA | 1.83 | 0.60 |
| 1:A:164:LYS:HB2 | 1:A:192:LEU:HA | 1.84 | 0.60 |
| 2:B:17:VAL:CG2 | 2:B:43:THR:HB | 2.31 | 0.60 |
| 1:A:217:GLU:HG3 | 1:A:221:ARG:NH1 | 2.15 | 0.60 |
| 1:A:232:TYR:O | 1:A:234:ASX:XD2 | 2.50 | 0.60 |
| 2:B:10:ALA:O | 2:B:11:GLU:HB3 | 2.02 | 0.60 |
| 1:A:272:VAL:O | 1:A:274:LYS:N | 2.34 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:14:ARG:HG2 | 2:B:64:THR:CG2 | 2.31 | 0.59 |
| 2:B:66:LEU:HB2 | 2:B:70:GLU:CB | 2.32 | 0.59 |
| 1:A:198:ILE:HD11 | 1:A:202:LEU:HD21 | 1.82 | 0.59 |
| 1:A:5:TYR:C | 1:A:7:SER:H | 2.05 | 0.59 |
| 2:B:140:CYS:SG | 2:B:140:CYS:O | 2.60 | 0.59 |
| 2:B:31:SER:O | 2:B:32:LEU:C | 2.38 | 0.59 |
| 2:B:69:ASP:HB2 | 2:B:72:ASP:CB | 2.32 | 0.59 |
| 1:A:110:GLY:O | 1:A:111:ALA:C | 2.40 | 0.59 |
| 1:A:194:MET:HG3 | 1:A:195:PRO:CD | 2.31 | 0.59 |
| 1:A:44:ILE:O | 1:A:71:VAL:HG23 | 2.00 | 0.59 |
| 1:A:136:THR:HG21 | 1:A:291:ARG:CZ | 2.32 | 0.59 |
| 1:A:31:LYS:HE3 | 1:A:143:PHE:HZ | 1.66 | 0.59 |
| 1:A:75:ASP:OD2 | 1:A:79:THR:HB | 2.03 | 0.59 |
| 1:A:12:ILE:HD13 | 1:A:175:ALA:HB2 | 1.84 | 0.59 |
| 1:A:29:LYS:CD | 1:A:29:LYS:H | 1.95 | 0.59 |
| 1:A:303:LEU:HD21 | 1:A:305:LEU:HD23 | 1.82 | 0.59 |
| 1:A:189:PRO:HD3 | 1:A:244:ASN:ND2 | 2.17 | 0.59 |
| 1:A:155:LEU:HD23 | 1:A:223:GLN:OE1 | 2.02 | 0.59 |
| 1:A:303:LEU:C | 1:A:303:LEU:CD2 | 2.66 | 0.59 |
| 1:A:39:LEU:O | 1:A:40:LYS:O | 2.21 | 0.59 |
| 2:B:85:ARG:HG2 | 2:B:90:GLU:HG2 | 1.84 | 0.59 |
| 1:A:178:LYS:O | 1:A:179:PHE:O | 2.21 | 0.59 |
| 2:B:128:ARG:NH1 | 2:B:143:GLU:OE2 | 2.27 | 0.59 |
| 2:B:18:ILE:HB | 2:B:44:ILE:HD13 | 1.85 | 0.59 |
| 1:A:157:VAL:CG1 | 1:A:184:PHE:HA | 2.33 | 0.58 |
| 1:A:208:ALA:HA | 1:A:209:TRP:CD1 | 2.33 | 0.58 |
| 1:A:303:LEU:CG | 1:A:305:LEU:HB3 | 2.32 | 0.58 |
| 2:B:44:ILE:HG22 | 2:B:45:GLY:H | 1.66 | 0.58 |
| 1:A:145:ILE:HG13 | 1:A:146:GLN:N | 2.18 | 0.58 |
| 1:A:171:SER:O | 1:A:172:LEU:C | 2.38 | 0.58 |
| 1:A:232:TYR:O | 1:A:234:ASX:N | 2.35 | 0.58 |
| 1:A:143:PHE:O | 1:A:146:GLN:CA | 2.50 | 0.58 |
| 2:B:116:SER:O | 2:B:117:HIS:HB2 | 2.00 | 0.58 |
| 2:B:145:SER:O | 2:B:147:ASN:CA | 2.50 | 0.58 |
| 2:B:66:LEU:C | 2:B:70:GLU:HG2 | 2.24 | 0.58 |
| 1:A:184:PHE:HE1 | 1:A:202:LEU:CD1 | 2.17 | 0.58 |
| 1:A:198:ILE:HG13 | 1:A:198:ILE:O | 2.03 | 0.58 |
| 1:A:138:THR:CG2 | 1:A:171:SER:HB2 | 2.34 | 0.58 |
| 1:A:281:PHE:O | 1:A:282:GLN:C | 2.42 | 0.58 |
| 1:A:8:HIS:N | 1:A:8:HIS:CD2 | 2.69 | 0.58 |
| 1:A:91:THR:O | 1:A:95:ILE:HB | 2.02 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:226:ARG:HH11 | 1:A:261:PRO:HD3 | 1.69 | 0.58 |
| 1:A:26:THR:HG21 | 1:A:297:LEU:HD11 | 1.84 | 0.58 |
| 2:B:72:ASP:OD2 | 2:B:98:SER:O | 2.22 | 0.58 |
| 1:A:201:MET:CB | 1:A:204:GLU:HG3 | 2.34 | 0.58 |
| 1:A:187:ILE:HD11 | 1:A:218:VAL:HG11 | 1.85 | 0.58 |
| 1:A:180:ASP:OD1 | 1:A:181:GLY:N | 2.37 | 0.58 |
| 2:B:25:ILE:CG1 | 2:B:25:ILE:O | 2.49 | 0.58 |
| 1:A:156:HIS:O | 1:A:223:GLN:HB2 | 2.03 | 0.58 |
| 1:A:226:ARG:NH1 | 1:A:261:PRO:HD3 | 2.19 | 0.58 |
| 2:B:47:ASN:O | 2:B:48:LEU:C | 2.42 | 0.58 |
| 1:A:182:ASN:OD1 | 1:A:182:ASN:N | 2.37 | 0.57 |
| 1:A:251:ASN:C | 1:A:253:LYS:H | 2.03 | 0.57 |
| 1:A:282:GLN:NE2 | 1:A:282:GLN:N | 2.09 | 0.57 |
| 2:B:12:ILE:O | 2:B:13:LYS:HG3 | 2.04 | 0.57 |
| 2:B:39:GLN:HE21 | 2:B:40:ASP:H | 1.50 | 0.57 |
| 1:A:49:PHE:CB | 1:A:105:ARG:O | 2.48 | 0.57 |
| 1:A:25:ALA:O | 1:A:26:THR:C | 2.40 | 0.57 |
| 2:B:102:ARG:O | 2:B:103:ASN:C | 2.40 | 0.57 |
| 2:B:129:ARG:O | 2:B:130:ALA:O | 2.22 | 0.57 |
| 2:B:76:LEU:HB3 | 2:B:77:TYR:CE1 | 2.38 | 0.57 |
| 1:A:200:ASP:O | 1:A:204:GLU:CB | 2.53 | 0.57 |
| 1:A:9:ILE:HB | 1:A:125:LEU:HD11 | 1.80 | 0.57 |
| 1:A:230:SER:O | 1:A:231:GLU:CD | 2.42 | 0.57 |
| 1:A:256:ALA:O | 1:A:257:LYS:HD2 | 2.05 | 0.57 |
| 2:B:31:SER:HG | 2:B:32:LEU:N | 2.02 | 0.57 |
| 1:A:192:LEU:O | 1:A:193:ALA:O | 2.22 | 0.57 |
| 1:A:303:LEU:CD2 | 1:A:305:LEU:HD22 | 2.35 | 0.57 |
| 1:A:49:PHE:HE1 | 1:A:104:MET:CE | 2.17 | 0.57 |
| 2:B:60:LYS:O | 2:B:61:ILE:HG13 | 2.04 | 0.57 |
| 1:A:81:LEU:HD22 | 1:A:82:GLY:C | 2.25 | 0.57 |
| 1:A:86:GLN:HG2 | 1:A:87:THR:H | 1.69 | 0.57 |
| 2:B:72:ASP:O | 2:B:75:ALA:HB3 | 2.04 | 0.57 |
| 2:B:138:LYS:O | 2:B:138:LYS:HG3 | 2.05 | 0.57 |
| 1:A:217:GLU:OE2 | 1:A:221:ARG:NH1 | 2.38 | 0.57 |
| 1:A:269:ALA:O | 1:A:270:THR:C | 2.43 | 0.57 |
| 1:A:40:LYS:C | 1:A:41:HIS:CD2 | 2.78 | 0.57 |
| 2:B:84:ASN:O | 2:B:92:VAL:CB | 2.53 | 0.57 |
| 1:A:270:THR:O | 1:A:273:ASP:HB2 | 2.05 | 0.56 |
| 1:A:41:HIS:N | 1:A:41:HIS:HD2 | 2.00 | 0.56 |
| 1:A:258:VAL:C | 1:A:259:LEU:HD12 | 2.26 | 0.56 |
| 1:A:234:ASX:HB1 | 1:A:238:GLN:HG2 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:20:HIS:O | 2:B:20:HIS:CD2 | 2.58 | 0.56 |
| 2:B:29:LEU:CD2 | 2:B:33:PHE:CE1 | 2.86 | 0.56 |
| 1:A:16:SER:O | 1:A:17:ARG:C | 2.44 | 0.56 |
| 1:A:138:THR:CG2 | 1:A:171:SER:CB | 2.77 | 0.56 |
| 2:B:114:CYS:SG | 2:B:137:CYS:SG | 3.04 | 0.56 |
| 2:B:146:HIS:HD2 | 2:B:147:ASN:CG | 2.09 | 0.56 |
| 2:B:29:LEU:CA | 2:B:32:LEU:HB3 | 2.35 | 0.56 |
| 2:B:72:ASP:OD1 | 2:B:98:SER:CA | 2.52 | 0.56 |
| 2:B:14:ARG:HG2 | 2:B:64:THR:HG23 | 1.88 | 0.56 |
| 1:A:11:SER:OG | 1:A:133:GLN:CD | 2.43 | 0.56 |
| 1:A:258:VAL:C | 1:A:259:LEU:HD13 | 2.26 | 0.56 |
| 2:B:32:LEU:HD23 | 2:B:106:VAL:HG21 | 1.84 | 0.56 |
| 1:A:144:THR:O | 1:A:145:ILE:C | 2.38 | 0.56 |
| 1:A:31:LYS:HG3 | 1:A:289:PHE:CZ | 2.41 | 0.56 |
| 2:B:108:VAL:O | 2:B:109:CYS:C | 2.45 | 0.56 |
| 2:B:115:ILE:O | 2:B:116:SER:C | 2.43 | 0.56 |
| 2:B:96:ARG:HB3 | 2:B:97:PRO:HD2 | 1.88 | 0.55 |
| 1:A:148:THR:OG1 | 1:A:149:GLU:N | 2.38 | 0.55 |
| 2:B:31:SER:HG | 2:B:32:LEU:H | 1.54 | 0.55 |
| 2:B:15:GLY:H | 2:B:64:THR:HG23 | 1.70 | 0.55 |
| 2:B:74:LEU:O | 2:B:75:ALA:C | 2.45 | 0.55 |
| 1:A:202:LEU:HB3 | 1:A:207:ILE:HG22 | 1.88 | 0.55 |
| 2:B:111:ASP:HB2 | 2:B:144:PHE:CZ | 2.40 | 0.55 |
| 2:B:118:ALA:C | 2:B:119:GLU:HG2 | 2.27 | 0.55 |
| 1:A:192:LEU:C | 1:A:193:ALA:O | 2.44 | 0.55 |
| 1:A:69:SER:C | 1:A:70:VAL:HG13 | 2.24 | 0.55 |
| 2:B:71:VAL:CA | 2:B:74:LEU:HD11 | 2.18 | 0.55 |
| 1:A:136:THR:CG2 | 1:A:291:ARG:CZ | 2.85 | 0.55 |
| 1:A:199:LEU:O | 1:A:200:ASP:C | 2.44 | 0.55 |
| 2:B:5:ASP:O | 2:B:6:LYS:HB2 | 2.06 | 0.55 |
| 2:B:32:LEU:HD13 | 2:B:77:TYR:HD2 | 1.72 | 0.55 |
| 1:A:262:LEU:CB | 1:A:263:PRO:CA | 2.83 | 0.55 |
| 1:A:29:LYS:HA | 1:A:32:ALA:HB3 | 1.88 | 0.55 |
| 1:A:160:VAL:O | 1:A:227:LEU:HA | 2.07 | 0.55 |
| 2:B:34:LYS:HB3 | 2:B:35:LEU:HD23 | 1.89 | 0.55 |
| 1:A:160:VAL:HG11 | 1:A:215:ILE:CD1 | 2.37 | 0.55 |
| 1:A:116:THR:O | 1:A:118:PHE:N | 2.40 | 0.54 |
| 1:A:165:TYR:CD2 | 1:A:165:TYR:N | 2.75 | 0.54 |
| 1:A:148:THR:OG1 | 1:A:224:LYS:HE3 | 2.07 | 0.54 |
| 1:A:294:LEU:O | 1:A:297:LEU:N | 2.40 | 0.54 |
| 1:A:10:ILE:O | 1:A:11:SER:HB2 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:9:ILE:HD12 | 1:A:125:LEU:HD11 | 1.89 | 0.54 |
| 1:A:14:ASP:OD2 | 1:A:113:ARG:NH2 | 2.40 | 0.54 |
| 1:A:141:ASP:OD1 | 1:A:226:ARG:NH1 | 2.38 | 0.54 |
| 1:A:303:LEU:CD1 | 1:A:305:LEU:CA | 2.68 | 0.54 |
| 2:B:71:VAL:HG12 | 2:B:97:PRO:HA | 1.89 | 0.54 |
| 1:A:157:VAL:HG21 | 1:A:159:MET:HE3 | 1.89 | 0.54 |
| 1:A:70:VAL:CA | 1:A:71:VAL:HG22 | 2.38 | 0.54 |
| 1:A:198:ILE:CD1 | 1:A:202:LEU:CD2 | 2.85 | 0.54 |
| 1:A:231:GLU:HB3 | 1:A:232:TYR:CE2 | 2.34 | 0.54 |
| 1:A:77:ALA:C | 1:A:79:THR:N | 2.61 | 0.54 |
| 2:B:114:CYS:SG | 2:B:140:CYS:SG | 3.05 | 0.54 |
| 1:A:11:SER:OG | 1:A:133:GLN:NE2 | 2.41 | 0.54 |
| 1:A:92:ILE:HA | 1:A:95:ILE:HG21 | 1.88 | 0.54 |
| 1:A:136:THR:HG21 | 1:A:291:ARG:NH2 | 2.22 | 0.54 |
| 2:B:9:VAL:CG2 | 2:B:14:ARG:O | 2.56 | 0.54 |
| 1:A:180:ASP:CG | 1:A:181:GLY:N | 2.62 | 0.54 |
| 2:B:28:LYS:O | 2:B:31:SER:N | 2.38 | 0.54 |
| 2:B:21:ILE:HG22 | 2:B:78:ALA:HB1 | 1.90 | 0.54 |
| 1:A:204:GLU:CD | 1:A:205:LYS:NZ | 2.61 | 0.54 |
| 1:A:211:LEU:O | 1:A:212:HIS:CG | 2.60 | 0.54 |
| 1:A:66:LEU:HG | 1:A:292:GLN:HG3 | 1.91 | 0.54 |
| 2:B:71:VAL:HA | 2:B:74:LEU:HD13 | 1.84 | 0.54 |
| 1:A:138:THR:HA | 1:A:141:ASP:HB2 | 1.90 | 0.53 |
| 2:B:74:LEU:CD2 | 2:B:97:PRO:HB3 | 2.37 | 0.53 |
| 2:B:81:ALA:C | 2:B:82:THR:OG1 | 2.46 | 0.53 |
| 1:A:68:ALA:O | 1:A:69:SER:CB | 2.54 | 0.53 |
| 1:A:190:ASP:OD1 | 1:A:190:ASP:N | 2.42 | 0.53 |
| 1:A:44:ILE:HG23 | 1:A:101:ALA:HB3 | 1.89 | 0.53 |
| 2:B:22:PRO:O | 2:B:22:PRO:CD | 2.51 | 0.53 |
| 2:B:47:ASN:O | 2:B:49:PRO:N | 2.41 | 0.53 |
| 1:A:11:SER:OG | 1:A:133:GLN:OE1 | 2.27 | 0.53 |
| 2:B:61:ILE:HG22 | 2:B:62:GLU:C | 2.29 | 0.53 |
| 1:A:146:GLN:O | 1:A:147:GLN:C | 2.47 | 0.53 |
| 1:A:187:ILE:CG2 | 1:A:214:SER:O | 2.55 | 0.53 |
| 1:A:88:LEU:O | 1:A:88:LEU:CG | 2.56 | 0.53 |
| 2:B:33:PHE:O | 2:B:34:LYS:C | 2.42 | 0.53 |
| 2:B:63:ASN:C | 2:B:64:THR:OG1 | 2.47 | 0.53 |
| 1:A:136:THR:CG2 | 1:A:291:ARG:HH21 | 2.17 | 0.53 |
| 1:A:160:VAL:HG11 | 1:A:215:ILE:HD13 | 1.91 | 0.53 |
| 1:A:142:LEU:O | 1:A:145:ILE:CG2 | 2.45 | 0.53 |
| 2:B:107:LEU:O | 2:B:108:VAL:CG1 | 2.52 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:84:ASN:C | 2:B:92:VAL:HG21 | 2.28 | 0.53 |
| 1:A:142:LEU:HD12 | 1:A:176:LEU:HD23 | 1.91 | 0.53 |
| 2:B:69:ASP:C | 2:B:71:VAL:N | 2.56 | 0.53 |
| 2:B:137:CYS:O | 2:B:138:LYS:C | 2.47 | 0.52 |
| 2:B:17:VAL:HG22 | 2:B:43:THR:N | 2.23 | 0.52 |
| 2:B:18:ILE:HD11 | 2:B:42:ILE:HG23 | 1.91 | 0.52 |
| 2:B:79:PRO:CG | 2:B:80:GLN:N | 2.70 | 0.52 |
| 2:B:36:THR:HG22 | 2:B:36:THR:O | 2.09 | 0.52 |
| 1:A:109:GLU:CA | 1:A:129:ASP:HB3 | 2.37 | 0.52 |
| 1:A:186:PHE:O | 1:A:188:ALA:N | 2.43 | 0.52 |
| 2:B:34:LYS:CG | 2:B:35:LEU:N | 2.38 | 0.52 |
| 2:B:119:GLU:HB2 | 2:B:120:PRO:CD | 2.38 | 0.52 |
| 1:A:132:ASN:HD21 | 2:B:141:GLU:CB | 2.18 | 0.52 |
| 1:A:5:TYR:CE2 | 1:A:301:ARG:HA | 2.45 | 0.52 |
| 2:B:131:ASP:O | 2:B:132:ASP:CG | 2.47 | 0.52 |
| 2:B:9:VAL:HG21 | 2:B:15:GLY:N | 2.24 | 0.52 |
| 2:B:86:ILE:H | 2:B:90:GLU:HB2 | 1.74 | 0.52 |
| 1:A:20:LEU:HD23 | 1:A:179:PHE:CE2 | 2.44 | 0.52 |
| 1:A:201:MET:CA | 1:A:204:GLU:HG3 | 2.35 | 0.52 |
| 1:A:140:LEU:CD1 | 1:A:286:ASN:C | 2.78 | 0.52 |
| 2:B:76:LEU:HB3 | 2:B:77:TYR:HD1 | 1.72 | 0.52 |
| 2:B:86:ILE:HG12 | 2:B:90:GLU:HB3 | 1.92 | 0.52 |
| 1:A:119:SER:O | 1:A:120:GLY:C | 2.43 | 0.52 |
| 2:B:39:GLN:H | 2:B:39:GLN:CD | 2.13 | 0.52 |
| 1:A:84:LYS:N | 1:A:84:LYS:HD2 | 2.25 | 0.52 |
| 2:B:39:GLN:CD | 2:B:39:GLN:N | 2.62 | 0.52 |
| 1:A:141:ASP:C | 1:A:144:THR:HG22 | 2.30 | 0.52 |
| 1:A:11:SER:OG | 2:B:141:GLU:OE1 | 2.28 | 0.52 |
| 1:A:56:ARG:HG2 | 1:A:56:ARG:O | 2.10 | 0.52 |
| 2:B:16:THR:HG22 | 2:B:17:VAL:H | 1.73 | 0.52 |
| 2:B:18:ILE:O | 2:B:44:ILE:HA | 2.10 | 0.52 |
| 1:A:60:GLN:C | 1:A:62:SER:N | 2.63 | 0.51 |
| 1:A:92:ILE:HA | 1:A:95:ILE:CG2 | 2.40 | 0.51 |
| 1:A:197:TYR:HA | 1:A:200:ASP:OD2 | 2.11 | 0.51 |
| 1:A:199:LEU:HA | 1:A:202:LEU:HD23 | 1.91 | 0.51 |
| 1:A:231:GLU:HA | 1:A:239:PHE:HZ | 1.74 | 0.51 |
| 2:B:17:VAL:CG2 | 2:B:43:THR:OG1 | 2.58 | 0.51 |
| 1:A:141:ASP:O | 1:A:144:THR:CG2 | 2.58 | 0.51 |
| 1:A:143:PHE:O | 1:A:145:ILE:N | 2.43 | 0.51 |
| 1:A:227:LEU:HD21 | 1:A:246:LEU:HB2 | 1.92 | 0.51 |
| 2:B:44:ILE:HG22 | 2:B:45:GLY:N | 2.25 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:194:MET:HE3 | 1:A:198:ILE:HG13 | 1.91 | 0.51 |
| 1:A:94:VAL:O | 1:A:95:ILE:C | 2.45 | 0.51 |
| 2:B:109:CYS:N | 2:B:125:PHE:HZ | 2.09 | 0.51 |
| 2:B:17:VAL:C | 2:B:18:ILE:HD12 | 2.30 | 0.51 |
| 1:A:251:ASN:CA | 1:A:253:LYS:HG3 | 2.41 | 0.51 |
| 1:A:281:PHE:C | 1:A:283:GLN:N | 2.56 | 0.51 |
| 2:B:14:ARG:HB2 | 2:B:40:ASP:CG | 2.31 | 0.51 |
| 2:B:15:GLY:C | 2:B:64:THR:OG1 | 2.49 | 0.51 |
| 1:A:148:THR:OG1 | 1:A:224:LYS:CE | 2.59 | 0.51 |
| 1:A:198:ILE:HD12 | 1:A:202:LEU:CD2 | 2.41 | 0.51 |
| 1:A:208:ALA:CA | 1:A:209:TRP:HD1 | 2.20 | 0.51 |
| 1:A:35:GLN:HG3 | 1:A:38:LEU:CD2 | 2.25 | 0.51 |
| 1:A:34:PRO:C | 1:A:35:GLN:NE2 | 2.64 | 0.51 |
| 2:B:128:ARG:CZ | 2:B:143:GLU:OE1 | 2.52 | 0.51 |
| 1:A:214:SER:CB | 1:A:216:GLU:HB2 | 2.37 | 0.51 |
| 1:A:124:VAL:HG23 | 1:A:125:LEU:O | 2.12 | 0.51 |
| 1:A:198:ILE:O | 1:A:199:LEU:CD1 | 2.42 | 0.51 |
| 1:A:258:VAL:HB | 1:A:277:HIS:O | 2.11 | 0.51 |
| 1:A:95:ILE:O | 1:A:96:SER:C | 2.49 | 0.51 |
| 2:B:99:LEU:CD1 | 2:B:127:VAL:HG11 | 2.40 | 0.51 |
| 1:A:13:ASN:O | 1:A:15:LEU:N | 2.38 | 0.50 |
| 1:A:224:LYS:HZ2 | 1:A:259:LEU:HD11 | 1.75 | 0.50 |
| 1:A:215:ILE:O | 1:A:219:MET:HB3 | 2.12 | 0.50 |
| 1:A:157:VAL:O | 1:A:185:TYR:CE1 | 2.58 | 0.50 |
| 1:A:211:LEU:O | 1:A:212:HIS:NE2 | 2.44 | 0.50 |
| 1:A:23:VAL:O | 1:A:24:LEU:C | 2.48 | 0.50 |
| 1:A:242:ARG:O | 1:A:242:ARG:HG3 | 2.12 | 0.50 |
| 1:A:93:SER:CA | 1:A:96:SER:OG | 2.58 | 0.50 |
| 2:B:29:LEU:O | 2:B:33:PHE:HD1 | 1.95 | 0.50 |
| 1:A:187:ILE:N | 1:A:187:ILE:HD12 | 2.22 | 0.50 |
| 2:B:146:HIS:CD2 | 2:B:147:ASN:CG | 2.84 | 0.50 |
| 2:B:148:VAL:O | 2:B:149:VAL:HG23 | 2.11 | 0.50 |
| 2:B:16:THR:HG22 | 2:B:17:VAL:N | 2.27 | 0.50 |
| 2:B:67:SER:HB3 | 2:B:70:GLU:HG2 | 1.94 | 0.50 |
| 2:B:9:VAL:HG22 | 2:B:14:ARG:C | 2.29 | 0.50 |
| 1:A:125:LEU:HD21 | 1:A:298:VAL:HG11 | 1.93 | 0.50 |
| 1:A:211:LEU:C | 1:A:212:HIS:CG | 2.84 | 0.50 |
| 1:A:291:ARG:O | 1:A:292:GLN:C | 2.49 | 0.50 |
| 1:A:80:SER:OG | 1:A:81:LEU:N | 2.33 | 0.50 |
| 2:B:71:VAL:HG13 | 2:B:74:LEU:CD2 | 2.36 | 0.50 |
| 1:A:136:THR:HG21 | 1:A:291:ARG:CG | 2.42 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:138:THR:OG1 | 1:A:139:LEU:N | 2.45 | 0.50 |
| 1:A:194:MET:CG | 1:A:195:PRO:HD2 | 2.39 | 0.50 |
| 1:A:267:GLU:OE1 | 1:A:267:GLU:N | 2.43 | 0.50 |
| 1:A:86:GLN:HG2 | 1:A:87:THR:N | 2.26 | 0.50 |
| 1:A:11:SER:HA | 1:A:133:GLN:OE1 | 2.11 | 0.50 |
| 1:A:141:ASP:CA | 1:A:144:THR:HG21 | 2.41 | 0.50 |
| 1:A:279:TRP:C | 1:A:281:PHE:H | 2.15 | 0.50 |
| 1:A:303:LEU:CD2 | 1:A:305:LEU:CD2 | 2.83 | 0.50 |
| 1:A:70:VAL:C | 1:A:71:VAL:CG2 | 2.58 | 0.50 |
| 1:A:199:LEU:H | 1:A:201:MET:H | 1.60 | 0.50 |
| 1:A:232:TYR:HD2 | 1:A:232:TYR:N | 2.08 | 0.50 |
| 1:A:227:LEU:HD13 | 1:A:268:ILE:CD1 | 2.41 | 0.50 |
| 1:A:289:PHE:O | 1:A:290:ALA:C | 2.50 | 0.50 |
| 1:A:136:THR:HG21 | 1:A:291:ARG:HG3 | 1.94 | 0.50 |
| 1:A:56:ARG:HD2 | 1:A:60:GLN:NE2 | 2.15 | 0.50 |
| 1:A:56:ARG:NE | 1:A:60:GLN:NE2 | 2.56 | 0.50 |
| 1:A:12:ILE:O | 1:A:13:ASN:C | 2.47 | 0.50 |
| 1:A:159:MET:HA | 1:A:226:ARG:O | 2.12 | 0.50 |
| 1:A:231:GLU:C | 1:A:232:TYR:CD2 | 2.86 | 0.50 |
| 2:B:20:HIS:CD2 | 2:B:20:HIS:C | 2.83 | 0.50 |
| 2:B:84:ASN:O | 2:B:92:VAL:CG1 | 2.60 | 0.50 |
| 1:A:43:VAL:HG13 | 1:A:43:VAL:O | 2.13 | 0.49 |
| 1:A:76:SER:O | 1:A:77:ALA:HB2 | 2.12 | 0.49 |
| 2:B:22:PRO:HD2 | 2:B:22:PRO:O | 2.11 | 0.49 |
| 1:A:11:SER:CB | 1:A:133:GLN:CD | 2.80 | 0.49 |
| 1:A:159:MET:HE2 | 1:A:172:LEU:HD23 | 1.93 | 0.49 |
| 2:B:72:ASP:O | 2:B:75:ALA:HB2 | 2.11 | 0.49 |
| 2:B:86:ILE:O | 2:B:90:GLU:CB | 2.59 | 0.49 |
| 2:B:91:VAL:O | 2:B:92:VAL:CG2 | 2.54 | 0.49 |
| 1:A:70:VAL:C | 1:A:71:VAL:HG13 | 2.29 | 0.49 |
| 2:B:36:THR:O | 2:B:36:THR:HG23 | 2.12 | 0.49 |
| 1:A:163:LEU:HD21 | 1:A:186:PHE:HB3 | 1.94 | 0.49 |
| 1:A:199:LEU:O | 1:A:203:ASP:N | 2.40 | 0.49 |
| 1:A:222:VAL:O | 1:A:254:MET:SD | 2.71 | 0.49 |
| 1:A:279:TRP:O | 1:A:281:PHE:C | 2.50 | 0.49 |
| 2:B:99:LEU:HD12 | 2:B:127:VAL:HG11 | 1.94 | 0.49 |
| 2:B:145:SER:O | 2:B:147:ASN:C | 2.50 | 0.49 |
| 2:B:63:ASN:HB3 | 2:B:84:ASN:CB | 2.43 | 0.49 |
| 2:B:9:VAL:HG11 | 2:B:15:GLY:N | 2.27 | 0.49 |
| 1:A:216:GLU:O | 1:A:219:MET:N | 2.46 | 0.49 |
| 2:B:33:PHE:CD1 | 2:B:33:PHE:N | 2.79 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:44:ILE:HG22 | 1:A:45:ALA:N | 2.26 | 0.49 |
| 2:B:145:SER:O | 2:B:147:ASN:O | 2.30 | 0.49 |
| 1:A:199:LEU:O | 1:A:202:LEU:N | 2.45 | 0.49 |
| 1:A:24:LEU:HD12 | 1:A:24:LEU:HA | 1.64 | 0.49 |
| 1:A:17:ARG:O | 1:A:20:LEU:N | 2.46 | 0.49 |
| 1:A:81:LEU:CD2 | 1:A:82:GLY:N | 2.60 | 0.49 |
| 1:A:9:ILE:O | 1:A:10:ILE:HD12 | 2.12 | 0.49 |
| 2:B:86:ILE:CG1 | 2:B:89:TYR:O | 2.41 | 0.49 |
| 1:A:111:ALA:O | 1:A:114:LEU:N | 2.46 | 0.49 |
| 1:A:185:TYR:C | 1:A:186:PHE:CD1 | 2.86 | 0.49 |
| 2:B:128:ARG:HG3 | 2:B:129:ARG:N | 2.27 | 0.49 |
| 2:B:86:ILE:H | 2:B:90:GLU:CG | 2.25 | 0.49 |
| 1:A:142:LEU:CD1 | 1:A:176:LEU:HD23 | 2.43 | 0.48 |
| 1:A:260:HIS:CD2 | 1:A:260:HIS:C | 2.84 | 0.48 |
| 1:A:60:GLN:O | 1:A:62:SER:N | 2.45 | 0.48 |
| 2:B:148:VAL:CG1 | 2:B:148:VAL:O | 2.56 | 0.48 |
| 1:A:120:GLY:O | 1:A:122:VAL:N | 2.45 | 0.48 |
| 1:A:4:LEU:O | 1:A:5:TYR:O | 2.32 | 0.48 |
| 2:B:32:LEU:HD13 | 2:B:77:TYR:CD2 | 2.48 | 0.48 |
| 2:B:60:LYS:O | 2:B:61:ILE:CG1 | 2.61 | 0.48 |
| 1:A:12:ILE:CG2 | 1:A:13:ASN:N | 2.76 | 0.48 |
| 1:A:201:MET:HG2 | 1:A:201:MET:O | 2.13 | 0.48 |
| 1:A:198:ILE:C | 1:A:199:LEU:HD12 | 2.31 | 0.48 |
| 2:B:138:LYS:O | 2:B:139:TYR:CG | 2.66 | 0.48 |
| 2:B:71:VAL:CG1 | 2:B:72:ASP:N | 2.53 | 0.48 |
| 2:B:75:ALA:CB | 2:B:99:LEU:N | 2.77 | 0.48 |
| 1:A:194:MET:HE3 | 1:A:198:ILE:CG1 | 2.43 | 0.48 |
| 1:A:264:ARG:HD3 | 1:A:268:ILE:HB | 1.95 | 0.48 |
| 2:B:134:ALA:C | 2:B:135:LEU:HD12 | 2.34 | 0.48 |
| 2:B:16:THR:C | 2:B:17:VAL:HG23 | 2.32 | 0.48 |
| 2:B:33:PHE:HB3 | 2:B:35:LEU:HD21 | 1.96 | 0.48 |
| 2:B:85:ARG:HG2 | 2:B:90:GLU:CG | 2.42 | 0.48 |
| 1:A:124:VAL:O | 1:A:125:LEU:HD13 | 2.13 | 0.48 |
| 1:A:17:ARG:HG3 | 1:A:18:ASP:N | 2.28 | 0.48 |
| 1:A:143:PHE:C | 1:A:145:ILE:N | 2.61 | 0.48 |
| 1:A:212:HIS:CD2 | 1:A:218:VAL:CG2 | 2.96 | 0.48 |
| 2:B:27:PHE:O | 2:B:30:LEU:N | 2.47 | 0.48 |
| 1:A:107:PRO:C | 1:A:108:GLN:O | 2.50 | 0.48 |
| 1:A:149:GLU:HG3 | 1:A:224:LYS:HG3 | 1.95 | 0.48 |
| 2:B:14:ARG:HB3 | 2:B:64:THR:HG23 | 1.95 | 0.48 |
| 2:B:86:ILE:H | 2:B:90:GLU:CB | 2.26 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:9:VAL:CG2 | 2:B:14:ARG:CA | 2.92 | 0.48 |
| 1:A:20:LEU:O | 1:A:24:LEU:CB | 2.35 | 0.48 |
| 1:A:63:MET:HG3 | 1:A:295:LEU:HD21 | 1.95 | 0.48 |
| 1:A:295:LEU:N | 1:A:298:VAL:HG23 | 2.26 | 0.48 |
| 2:B:146:HIS:HD2 | 2:B:147:ASN:N | 2.12 | 0.48 |
| 2:B:28:LYS:O | 2:B:32:LEU:CB | 2.59 | 0.48 |
| 2:B:113:ASN:O | 2:B:114:CYS:C | 2.53 | 0.47 |
| 2:B:84:ASN:O | 2:B:92:VAL:HG11 | 2.13 | 0.47 |
| 1:A:11:SER:HA | 1:A:133:GLN:CG | 2.44 | 0.47 |
| 1:A:201:MET:O | 1:A:202:LEU:C | 2.53 | 0.47 |
| 1:A:20:LEU:O | 1:A:24:LEU:HD22 | 2.13 | 0.47 |
| 1:A:198:ILE:CD1 | 1:A:202:LEU:HD21 | 2.44 | 0.47 |
| 1:A:231:GLU:HA | 1:A:239:PHE:CZ | 2.49 | 0.47 |
| 1:A:26:THR:HB | 1:A:297:LEU:HD11 | 1.96 | 0.47 |
| 1:A:29:LYS:O | 1:A:30:LEU:C | 2.52 | 0.47 |
| 1:A:227:LEU:HD11 | 1:A:246:LEU:HG | 1.97 | 0.47 |
| 1:A:192:LEU:HD13 | 1:A:192:LEU:N | 2.26 | 0.47 |
| 1:A:259:LEU:N | 1:A:259:LEU:HD12 | 2.28 | 0.47 |
| 1:A:48:PHE:CE2 | 1:A:56:ARG:HB2 | 2.49 | 0.47 |
| 1:A:260:HIS:CD2 | 1:A:262:LEU:HA | 2.49 | 0.47 |
| 1:A:31:LYS:HG2 | 1:A:31:LYS:O | 2.14 | 0.47 |
| 1:A:60:GLN:O | 1:A:63:MET:HB2 | 2.15 | 0.47 |
| 1:A:132:ASN:ND2 | 2:B:141:GLU:CB | 2.74 | 0.47 |
| 1:A:185:TYR:O | 1:A:186:PHE:HD1 | 1.98 | 0.47 |
| 2:B:27:PHE:O | 2:B:28:LYS:C | 2.52 | 0.47 |
| 1:A:137:GLN:HG2 | 1:A:168:THR:CG2 | 2.44 | 0.47 |
| 1:A:194:MET:CE | 1:A:198:ILE:CG1 | 2.91 | 0.47 |
| 1:A:83:LYS:O | 1:A:83:LYS:HG2 | 2.14 | 0.47 |
| 1:A:135:PRO:O | 1:A:139:LEU:CG | 2.61 | 0.47 |
| 1:A:281:PHE:O | 1:A:284:ALA:HB3 | 2.15 | 0.47 |
| 2:B:26:GLY:C | 2:B:30:LEU:HD12 | 2.35 | 0.47 |
| 2:B:86:ILE:CG1 | 2:B:90:GLU:HB3 | 2.45 | 0.47 |
| 1:A:157:VAL:HG13 | 1:A:184:PHE:HA | 1.97 | 0.46 |
| 1:A:20:LEU:HD23 | 1:A:179:PHE:HE2 | 1.79 | 0.46 |
| 1:A:251:ASN:HA | 1:A:253:LYS:HE3 | 1.97 | 0.46 |
| 1:A:264:ARG:HD2 | 1:A:268:ILE:O | 2.14 | 0.46 |
| 1:A:43:VAL:O | 1:A:43:VAL:CG1 | 2.63 | 0.46 |
| 2:B:76:LEU:C | 2:B:77:TYR:HD1 | 2.19 | 0.46 |
| 2:B:86:ILE:N | 2:B:90:GLU:CB | 2.78 | 0.46 |
| 2:B:8:GLN:O | 2:B:9:VAL:CG2 | 2.50 | 0.46 |
| 1:A:121:ASN:O | 1:A:122:VAL:HG22 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:230:SER:H | 1:A:231:GLU:CG | 2.24 | 0.46 |
| 1:A:51:ALA:HA | 1:A:74:SER:OG | 2.16 | 0.46 |
| 2:B:9:VAL:HG22 | 2:B:14:ARG:O | 2.14 | 0.46 |
| 1:A:112:ALA:O | 1:A:113:ARG:C | 2.52 | 0.46 |
| 1:A:163:LEU:HD22 | 1:A:188:ALA:CB | 2.46 | 0.46 |
| 2:B:84:ASN:CB | 2:B:92:VAL:HG21 | 2.44 | 0.46 |
| 1:A:200:ASP:O | 1:A:204:GLU:CA | 2.64 | 0.46 |
| 1:A:48:PHE:O | 1:A:49:PHE:C | 2.53 | 0.46 |
| 2:B:100:PRO:O | 2:B:101:GLU:CB | 2.63 | 0.46 |
| 2:B:102:ARG:CG | 2:B:102:ARG:O | 2.64 | 0.46 |
| 2:B:5:ASP:OD1 | 2:B:6:LYS:CA | 2.63 | 0.46 |
| 2:B:66:LEU:HD23 | 2:B:70:GLU:HB2 | 1.98 | 0.46 |
| 1:A:106:HIS:CD2 | 1:A:111:ALA:HB2 | 2.50 | 0.46 |
| 1:A:10:ILE:O | 1:A:11:SER:HB3 | 2.15 | 0.46 |
| 1:A:142:LEU:HA | 1:A:145:ILE:CG2 | 2.45 | 0.46 |
| 1:A:199:LEU:C | 1:A:201:MET:H | 2.16 | 0.46 |
| 1:A:204:GLU:CD | 1:A:205:LYS:HZ1 | 2.19 | 0.46 |
| 1:A:143:PHE:CE2 | 1:A:286:ASN:HB3 | 2.51 | 0.46 |
| 1:A:303:LEU:HD21 | 1:A:305:LEU:CB | 2.23 | 0.46 |
| 2:B:140:CYS:O | 2:B:142:LYS:N | 2.48 | 0.46 |
| 2:B:32:LEU:CD1 | 2:B:77:TYR:CD2 | 2.99 | 0.46 |
| 2:B:75:ALA:HB1 | 2:B:99:LEU:H | 1.81 | 0.46 |
| 1:A:185:TYR:O | 1:A:186:PHE:CD1 | 2.69 | 0.46 |
| 1:A:88:LEU:CD2 | 1:A:92:ILE:HG12 | 2.45 | 0.46 |
| 2:B:39:GLN:NE2 | 2:B:40:ASP:OD2 | 2.49 | 0.46 |
| 1:A:165:TYR:HD2 | 1:A:165:TYR:N | 2.13 | 0.46 |
| 1:A:261:PRO:C | 1:A:262:LEU:O | 2.54 | 0.46 |
| 2:B:99:LEU:HA | 2:B:100:PRO:HD3 | 1.65 | 0.46 |
| 2:B:14:ARG:HG2 | 2:B:64:THR:HG22 | 1.98 | 0.46 |
| 2:B:18:ILE:HG13 | 2:B:18:ILE:H | 1.00 | 0.46 |
| 2:B:1:MET:CG | 2:B:4:ASN:ND2 | 2.79 | 0.46 |
| 2:B:63:ASN:HB3 | 2:B:84:ASN:CA | 2.47 | 0.46 |
| 1:A:17:ARG:CG | 1:A:18:ASP:N | 2.79 | 0.45 |
| 2:B:44:ILE:CG2 | 2:B:45:GLY:H | 2.29 | 0.45 |
| 2:B:16:THR:HG22 | 2:B:18:ILE:HG13 | 1.98 | 0.45 |
| 2:B:23:ALA:O | 2:B:25:ILE:HG22 | 2.16 | 0.45 |
| 1:A:111:ALA:O | 1:A:112:ALA:O | 2.34 | 0.45 |
| 1:A:196:GLU:O | 1:A:200:ASP:CG | 2.55 | 0.45 |
| 1:A:218:VAL:O | 1:A:222:VAL:HG23 | 2.14 | 0.45 |
| 1:A:231:GLU:O | 1:A:234:ASX:XD1 | 2.64 | 0.45 |
| 1:A:284:ALA:C | 1:A:286:ASN:N | 2.68 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:9:ILE:HB | 1:A:125:LEU:HD13 | 1.89 | 0.45 |
| 2:B:61:ILE:CD1 | 2:B:82:THR:H | 2.26 | 0.45 |
| 2:B:86:ILE:CG2 | 2:B:90:GLU:CB | 2.84 | 0.45 |
| 1:A:152:LEU:HD13 | 1:A:179:PHE:CZ | 2.51 | 0.45 |
| 1:A:232:TYR:HB2 | 1:A:233:ALA:H | 1.38 | 0.45 |
| 1:A:279:TRP:HA | 1:A:282:GLN:HE22 | 1.77 | 0.45 |
| 1:A:288:ILE:C | 1:A:288:ILE:HD12 | 2.36 | 0.45 |
| 2:B:140:CYS:O | 2:B:142:LYS:HG2 | 2.16 | 0.45 |
| 1:A:227:LEU:O | 1:A:228:ASP:O | 2.33 | 0.45 |
| 2:B:83:VAL:HG23 | 2:B:92:VAL:HG13 | 1.97 | 0.45 |
| 1:A:172:LEU:O | 1:A:176:LEU:N | 2.40 | 0.45 |
| 1:A:202:LEU:HB3 | 1:A:207:ILE:CG2 | 2.46 | 0.45 |
| 1:A:199:LEU:O | 1:A:201:MET:N | 2.50 | 0.45 |
| 1:A:246:LEU:HD23 | 1:A:246:LEU:HA | 1.75 | 0.45 |
| 1:A:29:LYS:HB3 | 1:A:29:LYS:HE2 | 1.63 | 0.45 |
| 1:A:51:ALA:O | 1:A:52:SER:HB2 | 2.15 | 0.45 |
| 1:A:121:ASN:H | 1:A:121:ASN:ND2 | 2.15 | 0.45 |
| 1:A:11:SER:HA | 1:A:133:GLN:CD | 2.37 | 0.45 |
| 1:A:16:SER:O | 1:A:16:SER:OG | 2.35 | 0.45 |
| 2:B:62:GLU:CA | 2:B:62:GLU:OE1 | 2.65 | 0.45 |
| 1:A:156:HIS:CB | 1:A:223:GLN:HG3 | 2.47 | 0.45 |
| 2:B:113:ASN:HA | 2:B:113:ASN:HD22 | 1.68 | 0.45 |
| 2:B:140:CYS:O | 2:B:141:GLU:C | 2.55 | 0.45 |
| 1:A:187:ILE:HG23 | 1:A:213:SER:HA | 1.97 | 0.45 |
| 1:A:251:ASN:N | 1:A:253:LYS:HG3 | 2.32 | 0.45 |
| 1:A:260:HIS:HD2 | 1:A:262:LEU:N | 2.14 | 0.45 |
| 2:B:21:ILE:CG2 | 2:B:78:ALA:HB1 | 2.47 | 0.45 |
| 2:B:107:LEU:HD21 | 2:B:150:LEU:CD2 | 2.47 | 0.44 |
| 1:A:109:GLU:O | 2:B:139:TYR:O | 2.35 | 0.44 |
| 2:B:31:SER:O | 2:B:33:PHE:N | 2.50 | 0.44 |
| 2:B:14:ARG:CG | 2:B:64:THR:HG23 | 2.47 | 0.44 |
| 2:B:32:LEU:HD22 | 2:B:77:TYR:CE2 | 2.52 | 0.44 |
| 1:A:116:THR:O | 1:A:117:GLU:C | 2.55 | 0.44 |
| 1:A:217:GLU:HA | 1:A:217:GLU:OE1 | 2.11 | 0.44 |
| 1:A:218:VAL:O | 1:A:222:VAL:HG21 | 2.17 | 0.44 |
| 1:A:95:ILE:C | 1:A:99:VAL:CG2 | 2.82 | 0.44 |
| 2:B:9:VAL:CB | 2:B:14:ARG:HA | 2.40 | 0.44 |
| 1:A:294:LEU:O | 1:A:295:LEU:C | 2.56 | 0.44 |
| 1:A:44:ILE:CG2 | 1:A:45:ALA:H | 2.27 | 0.44 |
| 2:B:104:ILE:HD11 | 2:B:124:SER:OG | 2.17 | 0.44 |
| 2:B:21:ILE:HB | 2:B:22:PRO:CD | 2.39 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:173:THR:O | 1:A:177:ALA:N | 2.51 | 0.44 |
| 1:A:205:LYS:HZ3 | 1:A:205:LYS:HG2 | 1.34 | 0.44 |
| 1:A:225:GLU:O | 1:A:259:LEU:HB2 | 2.17 | 0.44 |
| 1:A:240:LEU:O | 1:A:242:ARG:N | 2.51 | 0.44 |
| 1:A:66:LEU:CG | 1:A:292:GLN:HG3 | 2.46 | 0.44 |
| 1:A:35:GLN:HB3 | 1:A:38:LEU:HD21 | 1.99 | 0.44 |
| 2:B:107:LEU:HD23 | 2:B:107:LEU:HA | 1.53 | 0.44 |
| 2:B:15:GLY:O | 2:B:64:THR:HG23 | 2.11 | 0.44 |
| 2:B:86:ILE:O | 2:B:90:GLU:HB3 | 2.18 | 0.44 |
| 1:A:109:GLU:HG2 | 1:A:132:ASN:HB3 | 2.00 | 0.44 |
| 1:A:46:SER:O | 1:A:72:GLY:HA3 | 2.17 | 0.44 |
| 2:B:128:ARG:HH11 | 2:B:143:GLU:CD | 1.90 | 0.44 |
| 1:A:192:LEU:N | 1:A:192:LEU:HD22 | 2.33 | 0.44 |
| 1:A:280:TYR:HA | 1:A:283:GLN:HE21 | 1.82 | 0.44 |
| 1:A:295:LEU:O | 1:A:299:LEU:HD12 | 2.18 | 0.44 |
| 2:B:19:ASN:O | 2:B:20:HIS:C | 2.56 | 0.44 |
| 1:A:135:PRO:O | 1:A:139:LEU:CD1 | 2.65 | 0.44 |
| 1:A:211:LEU:CA | 1:A:212:HIS:CE1 | 3.01 | 0.44 |
| 1:A:141:ASP:CG | 1:A:226:ARG:HH12 | 2.19 | 0.44 |
| 1:A:29:LYS:O | 1:A:31:LYS:N | 2.49 | 0.44 |
| 2:B:27:PHE:O | 2:B:30:LEU:HD12 | 2.18 | 0.44 |
| 2:B:7:LEU:HD13 | 2:B:63:ASN:HD22 | 1.83 | 0.44 |
| 1:A:11:SER:CA | 1:A:133:GLN:OE1 | 2.66 | 0.43 |
| 1:A:235:VAL:N | 1:A:238:GLN:HB3 | 2.32 | 0.43 |
| 1:A:24:LEU:HD11 | 1:A:143:PHE:HA | 2.01 | 0.43 |
| 1:A:71:VAL:CG2 | 1:A:71:VAL:O | 2.64 | 0.43 |
| 1:A:88:LEU:HD23 | 1:A:88:LEU:HA | 1.73 | 0.43 |
| 1:A:52:SER:HB2 | 1:A:105:ARG:HD3 | 2.01 | 0.43 |
| 1:A:143:PHE:O | 1:A:146:GLN:HB3 | 2.18 | 0.43 |
| 1:A:235:VAL:HB | 1:A:236:LYS:H | 1.37 | 0.43 |
| 1:A:166:GLY:O | 1:A:170:HIS:ND1 | 2.51 | 0.43 |
| 1:A:231:GLU:CA | 1:A:239:PHE:HZ | 2.32 | 0.43 |
| 1:A:76:SER:O | 1:A:77:ALA:HB3 | 2.15 | 0.43 |
| 2:B:71:VAL:CA | 2:B:74:LEU:CD1 | 2.77 | 0.43 |
| 1:A:202:LEU:HD13 | 1:A:207:ILE:HG21 | 1.96 | 0.43 |
| 1:A:219:MET:HE2 | 1:A:219:MET:O | 2.18 | 0.43 |
| 1:A:143:PHE:HE2 | 1:A:286:ASN:HB3 | 1.82 | 0.43 |
| 1:A:158:ALA:C | 1:A:159:MET:HG2 | 2.38 | 0.43 |
| 1:A:39:LEU:O | 1:A:42:LYS:HD2 | 2.18 | 0.43 |
| 2:B:106:VAL:CG1 | 2:B:106:VAL:O | 2.66 | 0.43 |
| 2:B:61:ILE:HG22 | 2:B:62:GLU:CB | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:157:VAL:HG22 | 1:A:158:ALA:N | 2.33 | 0.43 |
| 1:A:279:TRP:O | 1:A:282:GLN:N | 2.52 | 0.43 |
| 1:A:31:LYS:HG3 | 1:A:289:PHE:CE2 | 2.54 | 0.43 |
| 2:B:17:VAL:CA | 2:B:18:ILE:CD1 | 2.92 | 0.43 |
| 2:B:17:VAL:HG22 | 2:B:43:THR:CA | 2.48 | 0.43 |
| 1:A:175:ALA:C | 1:A:177:ALA:H | 2.20 | 0.43 |
| 1:A:303:LEU:CG | 1:A:305:LEU:N | 2.73 | 0.43 |
| 2:B:12:ILE:O | 2:B:13:LYS:HB2 | 2.17 | 0.43 |
| 2:B:138:LYS:O | 2:B:139:TYR:CD2 | 2.72 | 0.43 |
| 2:B:145:SER:C | 2:B:147:ASN:H | 2.21 | 0.43 |
| 2:B:4:ASN:ND2 | 2:B:5:ASP:O | 2.52 | 0.43 |
| 2:B:74:LEU:O | 2:B:77:TYR:N | 2.51 | 0.43 |
| 1:A:15:LEU:HA | 1:A:15:LEU:HD12 | 1.88 | 0.43 |
| 1:A:172:LEU:HA | 1:A:172:LEU:HD12 | 1.58 | 0.43 |
| 1:A:201:MET:HG3 | 1:A:204:GLU:OE1 | 2.18 | 0.43 |
| 1:A:216:GLU:HB3 | 1:A:217:GLU:H | 1.10 | 0.43 |
| 2:B:113:ASN:C | 2:B:114:CYS:O | 2.54 | 0.43 |
| 1:A:114:LEU:CD1 | 2:B:119:GLU:HG3 | 2.48 | 0.43 |
| 2:B:23:ALA:C | 2:B:25:ILE:HG22 | 2.39 | 0.43 |
| 1:A:59:PHE:CD1 | 1:A:103:VAL:HG21 | 2.53 | 0.43 |
| 1:A:121:ASN:HD22 | 1:A:121:ASN:H | 1.66 | 0.43 |
| 1:A:155:LEU:HD23 | 1:A:155:LEU:HA | 1.84 | 0.43 |
| 1:A:197:TYR:CE1 | 1:A:198:ILE:HG22 | 2.54 | 0.43 |
| 1:A:215:ILE:HG21 | 1:A:246:LEU:CD2 | 2.47 | 0.43 |
| 1:A:2:ASN:O | 1:A:3:PRO:C | 2.57 | 0.43 |
| 1:A:55:THR:HG22 | 1:A:55:THR:H | 1.55 | 0.43 |
| 1:A:92:ILE:O | 1:A:95:ILE:CG2 | 2.60 | 0.43 |
| 2:B:75:ALA:O | 2:B:79:PRO:HB3 | 2.18 | 0.43 |
| 2:B:107:LEU:HB3 | 2:B:125:PHE:HE1 | 1.82 | 0.42 |
| 1:A:106:HIS:HA | 1:A:107:PRO:HD3 | 1.64 | 0.42 |
| 2:B:73:GLU:OE1 | 2:B:100:PRO:HG2 | 2.18 | 0.42 |
| 1:A:112:ALA:O | 1:A:116:THR:N | 2.51 | 0.42 |
| 1:A:141:ASP:O | 1:A:144:THR:HG23 | 2.18 | 0.42 |
| 1:A:14:ASP:OD1 | 1:A:14:ASP:C | 2.55 | 0.42 |
| 1:A:80:SER:O | 1:A:81:LEU:CG | 2.67 | 0.42 |
| 2:B:102:ARG:O | 2:B:102:ARG:HG3 | 2.18 | 0.42 |
| 2:B:70:GLU:OE1 | 2:B:70:GLU:HA | 2.16 | 0.42 |
| 2:B:9:VAL:CG1 | 2:B:10:ALA:N | 2.78 | 0.42 |
| 1:A:240:LEU:HD22 | 1:A:241:VAL:H | 1.84 | 0.42 |
| 1:A:279:TRP:CD1 | 1:A:282:GLN:HB2 | 2.53 | 0.42 |
| 2:B:61:ILE:HD11 | 2:B:81:ALA:CB | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:14:ARG:CB | 2:B:64:THR:HG23 | 2.49 | 0.42 |
| 1:A:189:PRO:O | 1:A:190:ASP:C | 2.57 | 0.42 |
| 1:A:260:HIS:C | 1:A:262:LEU:N | 2.71 | 0.42 |
| 2:B:104:ILE:CG2 | 2:B:105:ASP:N | 2.83 | 0.42 |
| 2:B:146:HIS:NE2 | 2:B:147:ASN:OD1 | 2.53 | 0.42 |
| 2:B:30:LEU:HD21 | 2:B:44:ILE:CD1 | 2.49 | 0.42 |
| 2:B:64:THR:O | 2:B:65:PHE:HB3 | 2.20 | 0.42 |
| 1:A:151:ARG:CG | 1:A:151:ARG:HH11 | 2.33 | 0.42 |
| 1:A:253:LYS:O | 1:A:254:MET:HG2 | 2.20 | 0.42 |
| 1:A:274:LYS:HD3 | 1:A:275:THR:CA | 2.43 | 0.42 |
| 2:B:147:ASN:O | 2:B:149:VAL:CB | 2.66 | 0.42 |
| 1:A:189:PRO:HD3 | 1:A:244:ASN:HD21 | 1.85 | 0.42 |
| 1:A:49:PHE:HE1 | 1:A:104:MET:HE1 | 1.83 | 0.42 |
| 1:A:50:GLU:HG2 | 1:A:50:GLU:O | 2.18 | 0.42 |
| 1:A:52:SER:OG | 1:A:55:THR:CG2 | 2.64 | 0.42 |
| 1:A:184:PHE:HB3 | 1:A:186:PHE:CE1 | 2.55 | 0.42 |
| 1:A:227:LEU:HD13 | 1:A:268:ILE:HD11 | 2.02 | 0.42 |
| 2:B:61:ILE:CG1 | 2:B:82:THR:N | 2.57 | 0.42 |
| 2:B:72:ASP:O | 2:B:100:PRO:CG | 2.65 | 0.42 |
| 1:A:159:MET:HE2 | 1:A:172:LEU:CD2 | 2.50 | 0.41 |
| 1:A:149:GLU:CG | 1:A:224:LYS:HG3 | 2.50 | 0.41 |
| 1:A:279:TRP:HA | 1:A:282:GLN:CD | 2.39 | 0.41 |
| 1:A:303:LEU:CD1 | 1:A:305:LEU:CB | 2.94 | 0.41 |
| 2:B:61:ILE:CG2 | 2:B:62:GLU:CG | 2.86 | 0.41 |
| 2:B:85:ARG:HB3 | 2:B:90:GLU:HG3 | 2.02 | 0.41 |
| 1:A:227:LEU:HD11 | 1:A:246:LEU:CG | 2.50 | 0.41 |
| 1:A:284:ALA:O | 1:A:285:GLY:C | 2.57 | 0.41 |
| 2:B:15:GLY:N | 2:B:64:THR:HG23 | 2.35 | 0.41 |
| 2:B:67:SER:HB3 | 2:B:70:GLU:CG | 2.51 | 0.41 |
| 2:B:68:GLU:HB3 | 2:B:69:ASP:H | 1.44 | 0.41 |
| 1:A:8:HIS:CB | 1:A:10:ILE:CD1 | 2.80 | 0.41 |
| 2:B:75:ALA:CB | 2:B:99:LEU:H | 2.33 | 0.41 |
| 1:A:258:VAL:O | 1:A:259:LEU:HD12 | 2.19 | 0.41 |
| 1:A:75:ASP:OD1 | 1:A:79:THR:CB | 2.62 | 0.41 |
| 2:B:107:LEU:HA | 2:B:108:VAL:HG22 | 2.01 | 0.41 |
| 1:A:260:HIS:HA | 1:A:261:PRO:HD2 | 1.67 | 0.41 |
| 1:A:140:LEU:HD11 | 1:A:287:GLY:N | 2.36 | 0.41 |
| 1:A:291:ARG:O | 1:A:294:LEU:HB2 | 2.21 | 0.41 |
| 1:A:38:LEU:O | 1:A:39:LEU:HD23 | 2.20 | 0.41 |
| 1:A:60:GLN:C | 1:A:62:SER:H | 2.22 | 0.41 |
| 2:B:115:ILE:HG22 | 2:B:119:GLU:CG | 2.44 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:18:ILE:HD13 | 2:B:44:ILE:HG13 | 1.98 | 0.41 |
| 1:A:160:VAL:CG1 | 1:A:187:ILE:HG12 | 2.50 | 0.41 |
| 1:A:184:PHE:CD1 | 1:A:202:LEU:CD1 | 3.02 | 0.41 |
| 2:B:107:LEU:CB | 2:B:125:PHE:CE1 | 3.01 | 0.41 |
| 2:B:6:LYS:C | 2:B:8:GLN:H | 2.22 | 0.41 |
| 1:A:176:LEU:HA | 1:A:176:LEU:HD22 | 1.48 | 0.41 |
| 1:A:156:HIS:CE1 | 1:A:185:TYR:OH | 2.74 | 0.41 |
| 1:A:35:GLN:CB | 1:A:38:LEU:CD2 | 2.96 | 0.41 |
| 2:B:79:PRO:HG2 | 2:B:80:GLN:H | 1.84 | 0.41 |
| 2:B:11:GLU:O | 2:B:12:ILE:O | 2.38 | 0.41 |
| 2:B:14:ARG:HG2 | 2:B:64:THR:O | 2.20 | 0.41 |
| 2:B:69:ASP:CB | 2:B:72:ASP:HB2 | 2.41 | 0.41 |
| 2:B:63:ASN:CA | 2:B:84:ASN:HB2 | 2.41 | 0.41 |
| 1:A:20:LEU:HA | 1:A:20:LEU:HD12 | 1.85 | 0.41 |
| 1:A:282:GLN:O | 1:A:283:GLN:C | 2.58 | 0.41 |
| 1:A:38:LEU:N | 1:A:38:LEU:HD23 | 2.35 | 0.41 |
| 1:A:88:LEU:HD22 | 1:A:92:ILE:HG12 | 2.02 | 0.41 |
| 2:B:115:ILE:O | 2:B:118:ALA:N | 2.54 | 0.41 |
| 2:B:75:ALA:CB | 2:B:99:LEU:HA | 2.50 | 0.41 |
| 2:B:92:VAL:CG1 | 2:B:92:VAL:O | 2.62 | 0.40 |
| 1:A:12:ILE:HD11 | 1:A:138:THR:OG1 | 2.21 | 0.40 |
| 1:A:212:HIS:CD2 | 1:A:218:VAL:HG22 | 2.56 | 0.40 |
| 1:A:38:LEU:CB | 1:A:39:LEU:HD23 | 2.45 | 0.40 |
| 1:A:47:CYS:O | 1:A:104:MET:HA | 2.21 | 0.40 |
| 2:B:102:ARG:HH11 | 2:B:104:ILE:HD13 | 1.86 | 0.40 |
| 2:B:115:ILE:HG21 | 2:B:115:ILE:HD13 | 1.62 | 0.40 |
| 2:B:26:GLY:O | 2:B:30:LEU:HG | 2.21 | 0.40 |
| 1:A:141:ASP:CA | 1:A:144:THR:CG2 | 2.99 | 0.40 |
| 1:A:143:PHE:CG | 1:A:144:THR:N | 2.86 | 0.40 |
| 1:A:146:GLN:C | 1:A:148:THR:N | 2.74 | 0.40 |
| 1:A:215:ILE:HA | 1:A:215:ILE:HD13 | 1.79 | 0.40 |
| 1:A:228:ASP:N | 1:A:228:ASP:OD1 | 2.42 | 0.40 |
| 1:A:231:GLU:C | 1:A:232:TYR:O | 2.58 | 0.40 |
| 2:B:20:HIS:ND1 | 2:B:47:ASN:HB2 | 2.36 | 0.40 |
| 2:B:76:LEU:HD13 | 2:B:150:LEU:HD21 | 2.03 | 0.40 |
| 2:B:9:VAL:HG22 | 2:B:14:ARG:CA | 2.51 | 0.40 |
| 1:A:137:GLN:HG3 | 1:A:141:ASP:OD2 | 2.22 | 0.40 |
| 1:A:267:GLU:HB3 | 1:A:268:ILE:HG13 | 2.02 | 0.40 |
| 1:A:4:LEU:HA | 1:A:4:LEU:HD23 | 1.70 | 0.40 |
| 1:A:56:ARG:HD3 | 1:A:56:ARG:HH11 | 1.51 | 0.40 |
| 1:A:87:THR:O | 1:A:90:ASN:N | 2.55 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|----------------|--------------------------|-------------------|
| 1:A:254:MET:O | 1:A:255:ASN:CB | 2.70 | 0.40 |
| 2:B:17:VAL:HA | 2:B:43:THR:O | 2.20 | 0.40 |
| 2:B:86:ILE:CA | 2:B:90:GLU:CB | 3.00 | 0.40 |

All (16) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.





| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 2:B:3:HIS:CB | 2:B:4:ASN:O[6_555] | 0.69 | 1.51 |
| 2:B:3:HIS:O | 2:B:4:ASN:CB[6_555] | 0.71 | 1.49 |
| 2:B:3:HIS:C | 2:B:4:ASN:CA[6_555] | 0.72 | 1.48 |
| 2:B:3:HIS:O | 2:B:4:ASN:CA[6_555] | 1.03 | 1.17 |
| 2:B:4:ASN:N | 2:B:4:ASN:N[6_555] | 1.46 | 0.74 |
| 1:A:75:ASP:O | 1:A:78:ASN:OD1[3_555] | 1.46 | 0.74 |
| 2:B:3:HIS:CB | 2:B:4:ASN:C[6_555] | 1.50 | 0.70 |
| 1:A:54:ARG:NH2 | 1:A:86:GLN:NE2[3_555] | 1.67 | 0.53 |
| 2:B:3:HIS:CG | 2:B:4:ASN:O[6_555] | 1.76 | 0.44 |
| 2:B:3:HIS:C | 2:B:4:ASN:N[6_555] | 1.77 | 0.43 |
| 2:B:4:ASN:N | 2:B:4:ASN:CA[6_555] | 1.77 | 0.43 |
| 1:A:76:SER:C | 1:A:78:ASN:ND2[3_555] | 2.00 | 0.20 |
| 1:A:75:ASP:C | 1:A:78:ASN:OD1[3_555] | 2.06 | 0.14 |
| 1:A:76:SER:O | 1:A:78:ASN:ND2[3_555] | 2.11 | 0.09 |
| 1:A:76:SER:O | 1:A:78:ASN:CG[3_555] | 2.13 | 0.07 |
| 2:B:3:HIS:NE2 | 2:B:17:VAL:CG1[6_555] | 2.18 | 0.02 |

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 | 302/305 (99%) | 159 (53%) | 71 (24%) | 72 (24%) |   |
| 2 | B | 150/152 (99%) | 66 (44%) | 33 (22%) | 51 (34%) |   |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|---------------|-----------|-----------|-----------|-------------------|
| All | All | 452/457 (99%) | 225 (50%) | 104 (23%) | 123 (27%) | 0 0 |

All (123) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 5 | TYR |
| 1 | A | 6 | GLN |
| 1 | A | 10 | ILE |
| 1 | A | 11 | SER |
| 1 | A | 17 | ARG |
| 1 | A | 18 | ASP |
| 1 | A | 40 | LYS |
| 1 | A | 51 | ALA |
| 1 | A | 59 | PHE |
| 1 | A | 68 | ALA |
| 1 | A | 76 | SER |
| 1 | A | 77 | ALA |
| 1 | A | 78 | ASN |
| 1 | A | 81 | LEU |
| 1 | A | 88 | LEU |
| 1 | A | 111 | ALA |
| 1 | A | 116 | THR |
| 1 | A | 117 | GLU |
| 1 | A | 120 | GLY |
| 1 | A | 121 | ASN |
| 1 | A | 179 | PHE |
| 1 | A | 183 | ARG |
| 1 | A | 190 | ASP |
| 1 | A | 191 | ALA |
| 1 | A | 193 | ALA |
| 1 | A | 198 | ILE |
| 1 | A | 216 | GLU |
| 1 | A | 218 | VAL |
| 1 | A | 220 | THR |
| 1 | A | 228 | ASP |
| 1 | A | 232 | TYR |
| 1 | A | 237 | ALA |
| 1 | A | 241 | VAL |
| 1 | A | 252 | ALA |
| 1 | A | 254 | MET |
| 1 | A | 255 | ASN |
| 1 | A | 262 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 265 | VAL |
| 1 | A | 273 | ASP |
| 1 | A | 274 | LYS |
| 1 | A | 276 | PRO |
| 1 | A | 277 | HIS |
| 1 | A | 298 | VAL |
| 2 | B | 3 | HIS |
| 2 | B | 4 | ASN |
| 2 | B | 6 | LYS |
| 2 | B | 9 | VAL |
| 2 | B | 13 | LYS |
| 2 | B | 20 | HIS |
| 2 | B | 34 | LYS |
| 2 | B | 36 | THR |
| 2 | B | 58 | LEU |
| 2 | B | 61 | ILE |
| 2 | B | 64 | THR |
| 2 | B | 69 | ASP |
| 2 | B | 72 | ASP |
| 2 | B | 75 | ALA |
| 2 | B | 84 | ASN |
| 2 | B | 85 | ARG |
| 2 | B | 92 | VAL |
| 2 | B | 99 | LEU |
| 2 | B | 101 | GLU |
| 2 | B | 102 | ARG |
| 2 | B | 107 | LEU |
| 2 | B | 108 | VAL |
| 2 | B | 117 | HIS |
| 2 | B | 121 | VAL |
| 2 | B | 130 | ALA |
| 2 | B | 131 | ASP |
| 2 | B | 132 | ASP |
| 2 | B | 139 | TYR |
| 2 | B | 141 | GLU |
| 2 | B | 146 | HIS |
| 2 | B | 147 | ASN |
| 2 | B | 148 | VAL |
| 2 | B | 149 | VAL |
| 2 | B | 151 | ALA |
| 1 | A | 14 | ASP |
| 1 | A | 60 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 61 | THR |
| 1 | A | 181 | GLY |
| 1 | A | 187 | ILE |
| 1 | A | 209 | TRP |
| 1 | A | 229 | PRO |
| 1 | A | 264 | ARG |
| 1 | A | 279 | TRP |
| 1 | A | 280 | TYR |
| 1 | A | 292 | GLN |
| 1 | A | 294 | LEU |
| 2 | B | 11 | GLU |
| 2 | B | 12 | ILE |
| 2 | B | 17 | VAL |
| 2 | B | 22 | PRO |
| 2 | B | 67 | SER |
| 2 | B | 100 | PRO |
| 2 | B | 103 | ASN |
| 2 | B | 122 | SER |
| 1 | A | 37 | GLU |
| 1 | A | 233 | ALA |
| 1 | A | 235 | VAL |
| 1 | A | 267 | GLU |
| 1 | A | 291 | ARG |
| 1 | A | 293 | ALA |
| 2 | B | 26 | GLY |
| 2 | B | 28 | LYS |
| 2 | B | 38 | THR |
| 2 | B | 114 | CYS |
| 2 | B | 133 | ILE |
| 1 | A | 137 | GLN |
| 1 | A | 282 | GLN |
| 2 | B | 94 | LYS |
| 1 | A | 30 | LEU |
| 1 | A | 53 | THR |
| 1 | A | 71 | VAL |
| 1 | A | 143 | PHE |
| 1 | A | 148 | THR |
| 1 | A | 199 | LEU |
| 1 | A | 251 | ASN |
| 2 | B | 25 | ILE |
| 1 | A | 110 | GLY |
| 1 | A | 206 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 71 | VAL |
| 2 | B | 83 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|-----------|-------------|---|
| 1 | A | 254/254 (100%) | 136 (54%) | 118 (46%) | 0 | 0 |
| 2 | B | 126/136 (93%) | 70 (56%) | 56 (44%) | 0 | 0 |
| All | All | 380/390 (97%) | 206 (54%) | 174 (46%) | 0 | 0 |

All (174) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 2 | ASN |
| 1 | A | 5 | TYR |
| 1 | A | 12 | ILE |
| 1 | A | 13 | ASN |
| 1 | A | 14 | ASP |
| 1 | A | 15 | LEU |
| 1 | A | 16 | SER |
| 1 | A | 17 | ARG |
| 1 | A | 22 | LEU |
| 1 | A | 23 | VAL |
| 1 | A | 24 | LEU |
| 1 | A | 26 | THR |
| 1 | A | 29 | LYS |
| 1 | A | 35 | GLN |
| 1 | A | 36 | PRO |
| 1 | A | 38 | LEU |
| 1 | A | 39 | LEU |
| 1 | A | 42 | LYS |
| 1 | A | 46 | SER |
| 1 | A | 54 | ARG |
| 1 | A | 55 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 57 | LEU |
| 1 | A | 58 | SER |
| 1 | A | 59 | PHE |
| 1 | A | 60 | GLN |
| 1 | A | 62 | SER |
| 1 | A | 69 | SER |
| 1 | A | 70 | VAL |
| 1 | A | 71 | VAL |
| 1 | A | 74 | SER |
| 1 | A | 75 | ASP |
| 1 | A | 76 | SER |
| 1 | A | 81 | LEU |
| 1 | A | 83 | LYS |
| 1 | A | 84 | LYS |
| 1 | A | 88 | LEU |
| 1 | A | 95 | ILE |
| 1 | A | 96 | SER |
| 1 | A | 98 | TYR |
| 1 | A | 99 | VAL |
| 1 | A | 102 | ILE |
| 1 | A | 104 | MET |
| 1 | A | 116 | THR |
| 1 | A | 117 | GLU |
| 1 | A | 119 | SER |
| 1 | A | 121 | ASN |
| 1 | A | 122 | VAL |
| 1 | A | 125 | LEU |
| 1 | A | 133 | GLN |
| 1 | A | 145 | ILE |
| 1 | A | 147 | GLN |
| 1 | A | 151 | ARG |
| 1 | A | 153 | ASN |
| 1 | A | 156 | HIS |
| 1 | A | 159 | MET |
| 1 | A | 160 | VAL |
| 1 | A | 163 | LEU |
| 1 | A | 165 | TYR |
| 1 | A | 167 | ARG |
| 1 | A | 168 | THR |
| 1 | A | 176 | LEU |
| 1 | A | 178 | LYS |
| 1 | A | 179 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 182 | ASN |
| 1 | A | 187 | ILE |
| 1 | A | 190 | ASP |
| 1 | A | 192 | LEU |
| 1 | A | 194 | MET |
| 1 | A | 196 | GLU |
| 1 | A | 197 | TYR |
| 1 | A | 198 | ILE |
| 1 | A | 199 | LEU |
| 1 | A | 200 | ASP |
| 1 | A | 201 | MET |
| 1 | A | 204 | GLU |
| 1 | A | 205 | LYS |
| 1 | A | 207 | ILE |
| 1 | A | 211 | LEU |
| 1 | A | 217 | GLU |
| 1 | A | 219 | MET |
| 1 | A | 220 | THR |
| 1 | A | 221 | ARG |
| 1 | A | 222 | VAL |
| 1 | A | 225 | GLU |
| 1 | A | 226 | ARG |
| 1 | A | 227 | LEU |
| 1 | A | 228 | ASP |
| 1 | A | 232 | TYR |
| 1 | A | 235 | VAL |
| 1 | A | 236 | LYS |
| 1 | A | 238 | GLN |
| 1 | A | 240 | LEU |
| 1 | A | 241 | VAL |
| 1 | A | 245 | SER |
| 1 | A | 246 | LEU |
| 1 | A | 249 | LEU |
| 1 | A | 254 | MET |
| 1 | A | 255 | ASN |
| 1 | A | 257 | LYS |
| 1 | A | 259 | LEU |
| 1 | A | 264 | ARG |
| 1 | A | 270 | THR |
| 1 | A | 271 | ASP |
| 1 | A | 273 | ASP |
| 1 | A | 274 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 275 | THR |
| 1 | A | 276 | PRO |
| 1 | A | 279 | TRP |
| 1 | A | 280 | TYR |
| 1 | A | 282 | GLN |
| 1 | A | 286 | ASN |
| 1 | A | 297 | LEU |
| 1 | A | 298 | VAL |
| 1 | A | 300 | ASN |
| 1 | A | 301 | ARG |
| 1 | A | 303 | LEU |
| 1 | A | 304 | VAL |
| 1 | A | 305 | LEU |
| 2 | B | 5 | ASP |
| 2 | B | 6 | LYS |
| 2 | B | 8 | GLN |
| 2 | B | 14 | ARG |
| 2 | B | 18 | ILE |
| 2 | B | 20 | HIS |
| 2 | B | 22 | PRO |
| 2 | B | 24 | GLU |
| 2 | B | 25 | ILE |
| 2 | B | 31 | SER |
| 2 | B | 35 | LEU |
| 2 | B | 38 | THR |
| 2 | B | 46 | LEU |
| 2 | B | 61 | ILE |
| 2 | B | 62 | GLU |
| 2 | B | 63 | ASN |
| 2 | B | 66 | LEU |
| 2 | B | 67 | SER |
| 2 | B | 68 | GLU |
| 2 | B | 69 | ASP |
| 2 | B | 70 | GLU |
| 2 | B | 72 | ASP |
| 2 | B | 73 | GLU |
| 2 | B | 74 | LEU |
| 2 | B | 77 | TYR |
| 2 | B | 80 | GLN |
| 2 | B | 82 | THR |
| 2 | B | 85 | ARG |
| 2 | B | 86 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 87 | ASN |
| 2 | B | 88 | ASP |
| 2 | B | 89 | TYR |
| 2 | B | 90 | GLU |
| 2 | B | 102 | ARG |
| 2 | B | 104 | ILE |
| 2 | B | 105 | ASP |
| 2 | B | 108 | VAL |
| 2 | B | 109 | CYS |
| 2 | B | 113 | ASN |
| 2 | B | 114 | CYS |
| 2 | B | 116 | SER |
| 2 | B | 119 | GLU |
| 2 | B | 122 | SER |
| 2 | B | 123 | SER |
| 2 | B | 128 | ARG |
| 2 | B | 129 | ARG |
| 2 | B | 132 | ASP |
| 2 | B | 137 | CYS |
| 2 | B | 138 | LYS |
| 2 | B | 141 | GLU |
| 2 | B | 142 | LYS |
| 2 | B | 143 | GLU |
| 2 | B | 146 | HIS |
| 2 | B | 149 | VAL |
| 2 | B | 150 | LEU |
| 2 | B | 152 | ASN |

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 | 6 | GLN |
| 1 | A | 8 | HIS |
| 1 | A | 13 | ASN |
| 1 | A | 33 | ASN |
| 1 | A | 35 | GLN |
| 1 | A | 41 | HIS |
| 1 | A | 60 | GLN |
| 1 | A | 121 | ASN |
| 1 | A | 137 | GLN |
| 1 | A | 174 | GLN |
| 1 | A | 260 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 282 | GLN |
| 1 | A | 283 | GLN |
| 1 | A | 292 | GLN |
| 2 | B | 20 | HIS |
| 2 | B | 39 | GLN |
| 2 | B | 84 | ASN |
| 2 | B | 113 | ASN |
| 2 | B | 117 | HIS |
| 2 | B | 146 | HIS |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.