



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:29 AM GMT

PDB ID : 2MSP
Title : MAJOR SPERM PROTEIN, BETA ISOFORM, ENGINEERED C59S/T90C
MUTANT, PUTATIVE SUBFILAMENT STRUCTURE, PH 8.5
Authors : Bullock, T.L.; Mccoy, A.J.; Stewart, M.
Deposited on : 1997-12-19
Resolution : 3.30 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

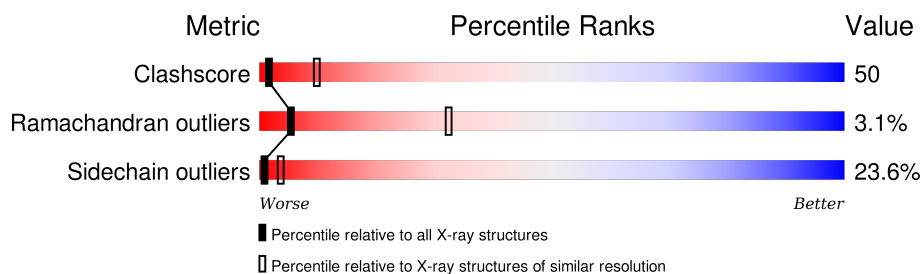
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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 | 102246 | 1058 (3.38-3.22) |
| Ramachandran outliers | 100387 | 1038 (3.38-3.22) |
| Sidechain outliers | 100360 | 1037 (3.38-3.22) |

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 | 126 | |
| 1 | B | 126 | |
| 1 | C | 126 | |
| 1 | D | 126 | |
| 1 | E | 126 | |
| 1 | F | 126 | |
| 1 | G | 126 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | H | 126 | <div><div></div><div>30%</div><div>49%</div><div>17%</div><div></div></div> |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7824 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 MAJOR SPERM PROTEIN.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1 | A | 124 | Total | C | N | O | S | 57 | 0 | 0 |
| | | | 978 | 610 | 178 | 185 | 5 | | | |
| 1 | B | 124 | Total | C | N | O | S | 57 | 0 | 0 |
| | | | 978 | 610 | 178 | 185 | 5 | | | |
| 1 | C | 124 | Total | C | N | O | S | 57 | 0 | 0 |
| | | | 978 | 610 | 178 | 185 | 5 | | | |
| 1 | D | 124 | Total | C | N | O | S | 57 | 0 | 0 |
| | | | 978 | 610 | 178 | 185 | 5 | | | |
| 1 | E | 124 | Total | C | N | O | S | 57 | 0 | 0 |
| | | | 978 | 610 | 178 | 185 | 5 | | | |
| 1 | F | 124 | Total | C | N | O | S | 57 | 0 | 0 |
| | | | 978 | 610 | 178 | 185 | 5 | | | |
| 1 | G | 124 | Total | C | N | O | S | 57 | 0 | 0 |
| | | | 978 | 610 | 178 | 185 | 5 | | | |
| 1 | H | 124 | Total | C | N | O | S | 51 | 0 | 0 |
| | | | 978 | 610 | 178 | 185 | 5 | | | |

There are 32 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------|------------|
| A | 59 | SER | CYS | ENGINEERED | UNP P27440 |
| A | 65 | SER | LYS | CONFLICT | UNP P27440 |
| A | 67 | LYS | SER | CONFLICT | UNP P27440 |
| A | 90 | CYS | THR | ENGINEERED | UNP P27440 |
| B | 59 | SER | CYS | ENGINEERED | UNP P27440 |
| B | 65 | SER | LYS | CONFLICT | UNP P27440 |
| B | 67 | LYS | SER | CONFLICT | UNP P27440 |
| B | 90 | CYS | THR | ENGINEERED | UNP P27440 |
| C | 59 | SER | CYS | ENGINEERED | UNP P27440 |
| C | 65 | SER | LYS | CONFLICT | UNP P27440 |
| C | 67 | LYS | SER | CONFLICT | UNP P27440 |
| C | 90 | CYS | THR | ENGINEERED | UNP P27440 |
| D | 59 | SER | CYS | ENGINEERED | UNP P27440 |

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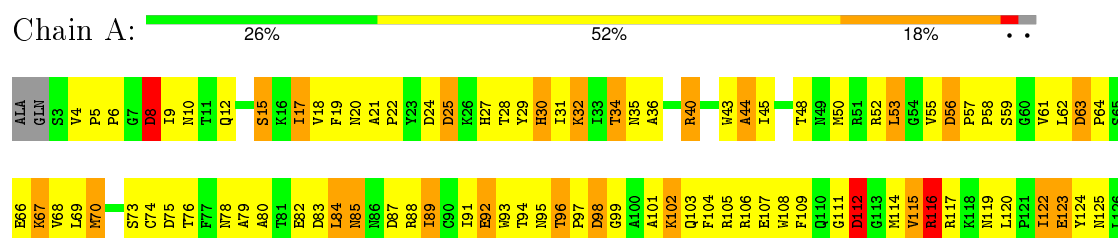
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------|------------|
| D | 65 | SER | LYS | CONFLICT | UNP P27440 |
| D | 67 | LYS | SER | CONFLICT | UNP P27440 |
| D | 90 | CYS | THR | ENGINEERED | UNP P27440 |
| E | 59 | SER | CYS | ENGINEERED | UNP P27440 |
| E | 65 | SER | LYS | CONFLICT | UNP P27440 |
| E | 67 | LYS | SER | CONFLICT | UNP P27440 |
| E | 90 | CYS | THR | ENGINEERED | UNP P27440 |
| F | 59 | SER | CYS | ENGINEERED | UNP P27440 |
| F | 65 | SER | LYS | CONFLICT | UNP P27440 |
| F | 67 | LYS | SER | CONFLICT | UNP P27440 |
| F | 90 | CYS | THR | ENGINEERED | UNP P27440 |
| G | 59 | SER | CYS | ENGINEERED | UNP P27440 |
| G | 65 | SER | LYS | CONFLICT | UNP P27440 |
| G | 67 | LYS | SER | CONFLICT | UNP P27440 |
| G | 90 | CYS | THR | ENGINEERED | UNP P27440 |
| H | 59 | SER | CYS | ENGINEERED | UNP P27440 |
| H | 65 | SER | LYS | CONFLICT | UNP P27440 |
| H | 67 | LYS | SER | CONFLICT | UNP P27440 |
| H | 90 | CYS | THR | ENGINEERED | UNP P27440 |

3 Residue-property plots [i](#)

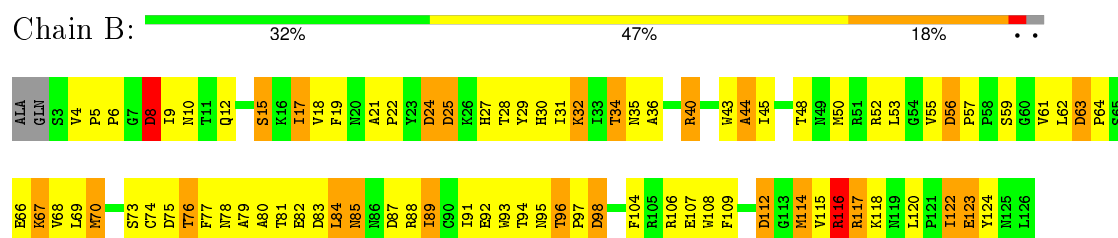
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

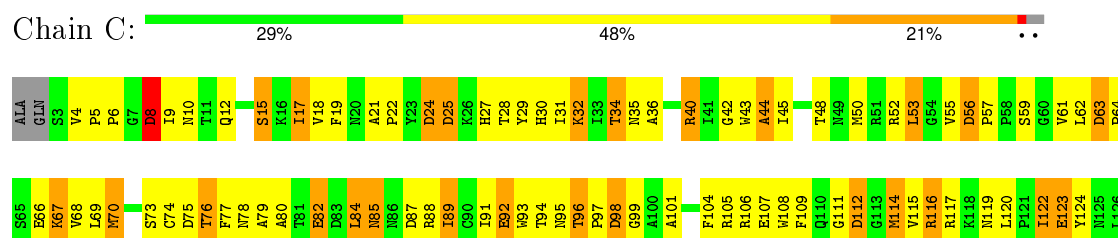
• Molecule 1: MAJOR SPERM PROTEIN



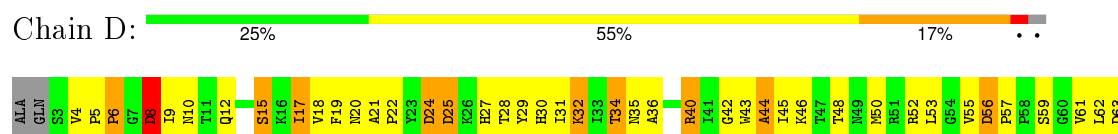
• Molecule 1: MAJOR SPERM PROTEIN

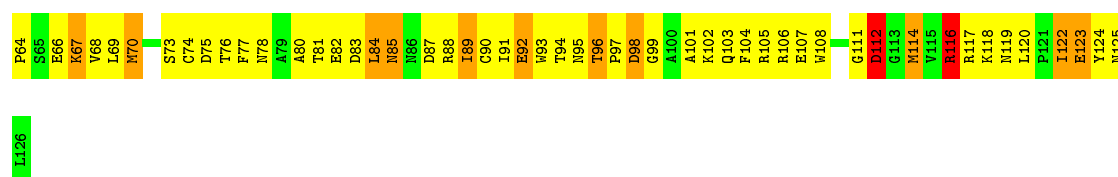


• Molecule 1: MAJOR SPERM PROTEIN

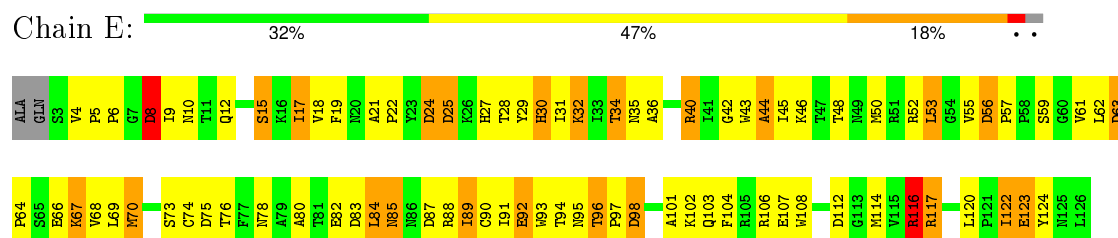


• Molecule 1: MAJOR SPERM PROTEIN

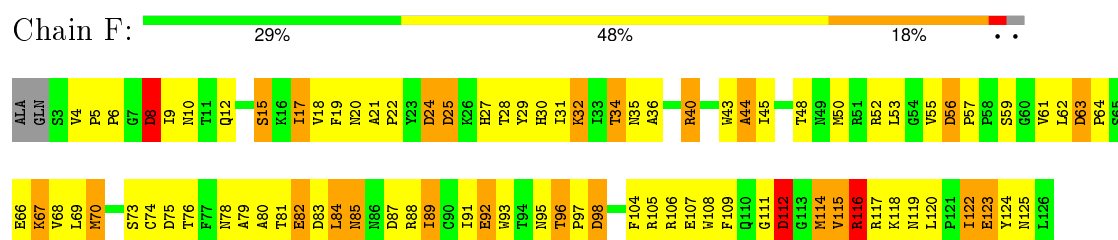




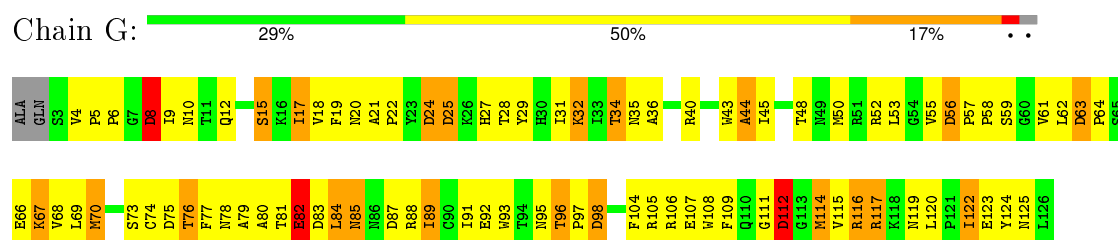
• Molecule 1: MAJOR SPERM PROTEIN



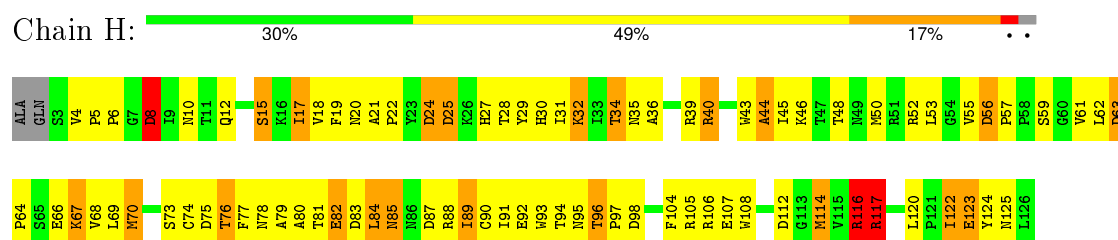
• Molecule 1: MAJOR SPERM PROTEIN



• Molecule 1: MAJOR SPERM PROTEIN



• Molecule 1: MAJOR SPERM PROTEIN



4 Data and refinement statistics

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

| Property | Value | Source |
|--|--|-----------|
| Space group | P 41 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 79.66 Å 79.66 Å 463.79 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 10.00 – 3.30 | Depositor |
| % Data completeness (in resolution range) | 100.0 (10.00-3.30) | Depositor |
| R_{merge} | 0.12 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | TNT V. 5-D | Depositor |
| R, R_{free} | 0.218 , 0.260 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 7824 | wwPDB-VP |
| Average B, all atoms (Å ²) | 50.0 | wwPDB-VP |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|------------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 1.30 | 5/1001 (0.5%) | 1.34 | 22/1358 (1.6%) |
| 1 | B | 1.31 | 5/1001 (0.5%) | 1.36 | 21/1358 (1.5%) |
| 1 | C | 1.30 | 6/1001 (0.6%) | 1.32 | 19/1358 (1.4%) |
| 1 | D | 1.31 | 5/1001 (0.5%) | 1.33 | 19/1358 (1.4%) |
| 1 | E | 1.30 | 5/1001 (0.5%) | 1.36 | 20/1358 (1.5%) |
| 1 | F | 1.29 | 5/1001 (0.5%) | 1.34 | 22/1358 (1.6%) |
| 1 | G | 1.29 | 6/1001 (0.6%) | 1.32 | 20/1358 (1.5%) |
| 1 | H | 1.28 | 5/1001 (0.5%) | 1.35 | 22/1358 (1.6%) |
| All | All | 1.30 | 42/8008 (0.5%) | 1.34 | 165/10864 (1.5%) |

All (42) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | F | 82 | GLU | CD-OE2 | 7.36 | 1.33 | 1.25 |
| 1 | D | 66 | GLU | CD-OE2 | 7.22 | 1.33 | 1.25 |
| 1 | D | 82 | GLU | CD-OE2 | 7.03 | 1.33 | 1.25 |
| 1 | A | 82 | GLU | CD-OE2 | 6.91 | 1.33 | 1.25 |
| 1 | B | 82 | GLU | CD-OE2 | 6.87 | 1.33 | 1.25 |
| 1 | E | 107 | GLU | CD-OE1 | 6.76 | 1.33 | 1.25 |
| 1 | F | 92 | GLU | CD-OE2 | 6.76 | 1.33 | 1.25 |
| 1 | H | 82 | GLU | CD-OE2 | 6.76 | 1.33 | 1.25 |
| 1 | H | 107 | GLU | CD-OE1 | 6.74 | 1.33 | 1.25 |
| 1 | F | 66 | GLU | CD-OE2 | 6.71 | 1.33 | 1.25 |
| 1 | D | 123 | GLU | CD-OE2 | 6.65 | 1.32 | 1.25 |
| 1 | A | 123 | GLU | CD-OE2 | 6.64 | 1.32 | 1.25 |
| 1 | G | 107 | GLU | CD-OE1 | 6.63 | 1.32 | 1.25 |
| 1 | B | 92 | GLU | CD-OE2 | 6.53 | 1.32 | 1.25 |
| 1 | C | 66 | GLU | CD-OE2 | 6.52 | 1.32 | 1.25 |
| 1 | C | 82 | GLU | CD-OE2 | 6.50 | 1.32 | 1.25 |
| 1 | E | 82 | GLU | CD-OE2 | 6.40 | 1.32 | 1.25 |
| 1 | G | 82 | GLU | CD-OE1 | 6.38 | 1.32 | 1.25 |
| 1 | E | 123 | GLU | CD-OE2 | 6.38 | 1.32 | 1.25 |
| 1 | D | 107 | GLU | CD-OE1 | 6.34 | 1.32 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 107 | GLU | CD-OE1 | 6.32 | 1.32 | 1.25 |
| 1 | C | 123 | GLU | CD-OE2 | 6.31 | 1.32 | 1.25 |
| 1 | H | 92 | GLU | CD-OE2 | 6.20 | 1.32 | 1.25 |
| 1 | F | 107 | GLU | CD-OE1 | 6.19 | 1.32 | 1.25 |
| 1 | G | 66 | GLU | CD-OE2 | 6.16 | 1.32 | 1.25 |
| 1 | B | 123 | GLU | CD-OE2 | 6.13 | 1.32 | 1.25 |
| 1 | E | 66 | GLU | CD-OE2 | 6.00 | 1.32 | 1.25 |
| 1 | C | 107 | GLU | CD-OE1 | 5.97 | 1.32 | 1.25 |
| 1 | G | 82 | GLU | CD-OE2 | -5.85 | 1.19 | 1.25 |
| 1 | H | 66 | GLU | CD-OE2 | 5.83 | 1.32 | 1.25 |
| 1 | F | 123 | GLU | CD-OE2 | 5.81 | 1.32 | 1.25 |
| 1 | B | 66 | GLU | CD-OE2 | 5.80 | 1.32 | 1.25 |
| 1 | G | 92 | GLU | CD-OE2 | 5.71 | 1.31 | 1.25 |
| 1 | A | 66 | GLU | CD-OE2 | 5.66 | 1.31 | 1.25 |
| 1 | B | 107 | GLU | CD-OE1 | 5.56 | 1.31 | 1.25 |
| 1 | E | 92 | GLU | CD-OE2 | 5.56 | 1.31 | 1.25 |
| 1 | H | 123 | GLU | CD-OE2 | 5.54 | 1.31 | 1.25 |
| 1 | C | 92 | GLU | CD-OE2 | 5.44 | 1.31 | 1.25 |
| 1 | G | 123 | GLU | CD-OE2 | 5.33 | 1.31 | 1.25 |
| 1 | D | 92 | GLU | CD-OE2 | 5.28 | 1.31 | 1.25 |
| 1 | A | 92 | GLU | CD-OE2 | 5.18 | 1.31 | 1.25 |
| 1 | C | 101 | ALA | C-N | -5.04 | 1.22 | 1.34 |

All (165) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | E | 112 | ASP | CB-CG-OD2 | -9.63 | 109.63 | 118.30 |
| 1 | H | 112 | ASP | CB-CG-OD1 | 8.09 | 125.58 | 118.30 |
| 1 | B | 112 | ASP | CB-CG-OD1 | 8.02 | 125.52 | 118.30 |
| 1 | H | 112 | ASP | CB-CG-OD2 | -7.97 | 111.13 | 118.30 |
| 1 | H | 117 | ARG | NE-CZ-NH2 | -7.66 | 116.47 | 120.30 |
| 1 | A | 112 | ASP | CB-CG-OD2 | -7.63 | 111.44 | 118.30 |
| 1 | A | 24 | ASP | CB-CG-OD2 | -7.45 | 111.60 | 118.30 |
| 1 | G | 112 | ASP | CB-CG-OD2 | -7.41 | 111.63 | 118.30 |
| 1 | B | 117 | ARG | NE-CZ-NH2 | -7.28 | 116.66 | 120.30 |
| 1 | G | 112 | ASP | CB-CG-OD1 | 7.21 | 124.79 | 118.30 |
| 1 | C | 112 | ASP | CB-CG-OD1 | 7.17 | 124.75 | 118.30 |
| 1 | C | 112 | ASP | CB-CG-OD2 | -7.07 | 111.94 | 118.30 |
| 1 | B | 112 | ASP | CB-CG-OD2 | -7.01 | 111.99 | 118.30 |
| 1 | H | 44 | ALA | N-CA-CB | 6.99 | 119.89 | 110.10 |
| 1 | F | 112 | ASP | CB-CG-OD1 | 6.99 | 124.59 | 118.30 |
| 1 | G | 8 | ASP | CB-CG-OD2 | -6.93 | 112.06 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 112 | ASP | CB-CG-OD1 | 6.86 | 124.48 | 118.30 |
| 1 | E | 44 | ALA | N-CA-CB | 6.85 | 119.69 | 110.10 |
| 1 | F | 56 | ASP | CB-CG-OD2 | -6.78 | 112.20 | 118.30 |
| 1 | B | 44 | ALA | N-CA-CB | 6.71 | 119.49 | 110.10 |
| 1 | C | 8 | ASP | CB-CG-OD2 | -6.68 | 112.29 | 118.30 |
| 1 | F | 56 | ASP | CB-CG-OD1 | 6.67 | 124.30 | 118.30 |
| 1 | F | 44 | ALA | N-CA-CB | 6.64 | 119.40 | 110.10 |
| 1 | A | 8 | ASP | CB-CG-OD2 | -6.63 | 112.33 | 118.30 |
| 1 | F | 8 | ASP | CB-CG-OD2 | -6.62 | 112.34 | 118.30 |
| 1 | D | 44 | ALA | N-CA-CB | 6.61 | 119.36 | 110.10 |
| 1 | F | 25 | ASP | CB-CG-OD2 | -6.60 | 112.36 | 118.30 |
| 1 | E | 8 | ASP | CB-CG-OD2 | -6.58 | 112.38 | 118.30 |
| 1 | D | 8 | ASP | CB-CG-OD2 | -6.58 | 112.38 | 118.30 |
| 1 | B | 8 | ASP | CB-CG-OD2 | -6.54 | 112.42 | 118.30 |
| 1 | E | 117 | ARG | NE-CZ-NH2 | -6.53 | 117.04 | 120.30 |
| 1 | C | 44 | ALA | CB-CA-C | 6.52 | 119.88 | 110.10 |
| 1 | A | 44 | ALA | N-CA-CB | 6.51 | 119.21 | 110.10 |
| 1 | H | 25 | ASP | CB-CG-OD2 | -6.49 | 112.46 | 118.30 |
| 1 | F | 44 | ALA | CB-CA-C | 6.48 | 119.82 | 110.10 |
| 1 | H | 8 | ASP | CB-CG-OD2 | -6.45 | 112.50 | 118.30 |
| 1 | G | 44 | ALA | N-CA-CB | 6.44 | 119.11 | 110.10 |
| 1 | A | 98 | ASP | CB-CG-OD2 | -6.39 | 112.55 | 118.30 |
| 1 | F | 83 | ASP | CB-CG-OD2 | -6.36 | 112.57 | 118.30 |
| 1 | D | 56 | ASP | CB-CG-OD2 | -6.36 | 112.58 | 118.30 |
| 1 | B | 25 | ASP | CB-CG-OD2 | -6.35 | 112.59 | 118.30 |
| 1 | C | 56 | ASP | CB-CG-OD2 | -6.28 | 112.65 | 118.30 |
| 1 | H | 56 | ASP | CB-CG-OD1 | 6.27 | 123.94 | 118.30 |
| 1 | C | 44 | ALA | N-CA-CB | 6.26 | 118.87 | 110.10 |
| 1 | E | 44 | ALA | CB-CA-C | 6.26 | 119.50 | 110.10 |
| 1 | H | 24 | ASP | CB-CG-OD2 | -6.26 | 112.67 | 118.30 |
| 1 | F | 24 | ASP | CB-CG-OD2 | -6.26 | 112.67 | 118.30 |
| 1 | B | 44 | ALA | CB-CA-C | 6.22 | 119.44 | 110.10 |
| 1 | A | 44 | ALA | CB-CA-C | 6.22 | 119.43 | 110.10 |
| 1 | B | 87 | ASP | CB-CG-OD1 | -6.17 | 112.75 | 118.30 |
| 1 | D | 44 | ALA | CB-CA-C | 6.17 | 119.36 | 110.10 |
| 1 | H | 87 | ASP | CB-CG-OD2 | 6.15 | 123.84 | 118.30 |
| 1 | E | 98 | ASP | CB-CG-OD2 | -6.11 | 112.80 | 118.30 |
| 1 | C | 56 | ASP | CB-CG-OD1 | 6.11 | 123.80 | 118.30 |
| 1 | H | 87 | ASP | CB-CG-OD1 | -6.06 | 112.85 | 118.30 |
| 1 | E | 24 | ASP | CB-CG-OD2 | -6.05 | 112.85 | 118.30 |
| 1 | G | 25 | ASP | CB-CG-OD2 | -6.05 | 112.85 | 118.30 |
| 1 | E | 116 | ARG | NE-CZ-NH2 | -6.05 | 117.27 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | D | 83 | ASP | CB-CG-OD2 | -6.05 | 112.86 | 118.30 |
| 1 | G | 44 | ALA | CB-CA-C | 6.03 | 119.14 | 110.10 |
| 1 | E | 56 | ASP | CB-CG-OD2 | -6.03 | 112.88 | 118.30 |
| 1 | B | 116 | ARG | NE-CZ-NH1 | 6.02 | 123.31 | 120.30 |
| 1 | D | 56 | ASP | CB-CG-OD1 | 6.02 | 123.72 | 118.30 |
| 1 | B | 24 | ASP | CB-CG-OD2 | -6.02 | 112.88 | 118.30 |
| 1 | B | 98 | ASP | CB-CG-OD2 | -5.99 | 112.91 | 118.30 |
| 1 | E | 25 | ASP | CB-CG-OD2 | -5.98 | 112.92 | 118.30 |
| 1 | C | 24 | ASP | CB-CG-OD2 | -5.94 | 112.95 | 118.30 |
| 1 | H | 98 | ASP | CB-CG-OD2 | -5.94 | 112.95 | 118.30 |
| 1 | D | 24 | ASP | CB-CG-OD2 | -5.93 | 112.96 | 118.30 |
| 1 | C | 25 | ASP | CB-CG-OD2 | -5.93 | 112.96 | 118.30 |
| 1 | H | 56 | ASP | CB-CG-OD2 | -5.93 | 112.97 | 118.30 |
| 1 | E | 87 | ASP | CB-CG-OD2 | 5.92 | 123.63 | 118.30 |
| 1 | D | 87 | ASP | CB-CG-OD2 | 5.92 | 123.63 | 118.30 |
| 1 | G | 56 | ASP | CB-CG-OD2 | -5.92 | 112.97 | 118.30 |
| 1 | F | 98 | ASP | CB-CG-OD2 | -5.91 | 112.98 | 118.30 |
| 1 | B | 56 | ASP | CB-CG-OD1 | 5.91 | 123.62 | 118.30 |
| 1 | D | 25 | ASP | CB-CG-OD2 | -5.91 | 112.98 | 118.30 |
| 1 | A | 83 | ASP | CB-CG-OD2 | -5.91 | 112.98 | 118.30 |
| 1 | A | 87 | ASP | CB-CG-OD2 | 5.90 | 123.61 | 118.30 |
| 1 | G | 75 | ASP | CB-CG-OD2 | -5.90 | 112.99 | 118.30 |
| 1 | F | 75 | ASP | CB-CG-OD2 | -5.89 | 113.00 | 118.30 |
| 1 | A | 87 | ASP | CB-CG-OD1 | -5.89 | 113.00 | 118.30 |
| 1 | D | 87 | ASP | CB-CG-OD1 | -5.86 | 113.02 | 118.30 |
| 1 | D | 75 | ASP | CB-CG-OD2 | -5.85 | 113.03 | 118.30 |
| 1 | G | 56 | ASP | CB-CG-OD1 | 5.84 | 123.56 | 118.30 |
| 1 | B | 87 | ASP | CB-CG-OD2 | 5.83 | 123.55 | 118.30 |
| 1 | E | 56 | ASP | CB-CG-OD1 | 5.83 | 123.55 | 118.30 |
| 1 | D | 112 | ASP | CB-CG-OD1 | 5.83 | 123.55 | 118.30 |
| 1 | F | 83 | ASP | CB-CG-OD1 | 5.83 | 123.55 | 118.30 |
| 1 | H | 75 | ASP | CB-CG-OD2 | -5.83 | 113.06 | 118.30 |
| 1 | C | 75 | ASP | CB-CG-OD2 | -5.81 | 113.07 | 118.30 |
| 1 | A | 56 | ASP | CB-CG-OD2 | -5.79 | 113.09 | 118.30 |
| 1 | G | 117 | ARG | NE-CZ-NH1 | 5.79 | 123.19 | 120.30 |
| 1 | E | 87 | ASP | CB-CG-OD1 | -5.77 | 113.11 | 118.30 |
| 1 | A | 112 | ASP | N-CA-CB | 5.77 | 120.99 | 110.60 |
| 1 | D | 98 | ASP | CB-CG-OD2 | -5.75 | 113.13 | 118.30 |
| 1 | A | 56 | ASP | CB-CG-OD1 | 5.73 | 123.46 | 118.30 |
| 1 | A | 25 | ASP | CB-CG-OD2 | -5.72 | 113.15 | 118.30 |
| 1 | G | 98 | ASP | CB-CG-OD2 | -5.72 | 113.15 | 118.30 |
| 1 | B | 75 | ASP | CB-CG-OD2 | -5.71 | 113.16 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | F | 117 | ARG | NE-CZ-NH1 | 5.71 | 123.15 | 120.30 |
| 1 | H | 44 | ALA | CB-CA-C | 5.70 | 118.65 | 110.10 |
| 1 | H | 83 | ASP | CB-CG-OD2 | -5.70 | 113.17 | 118.30 |
| 1 | C | 98 | ASP | CB-CG-OD2 | -5.68 | 113.19 | 118.30 |
| 1 | B | 116 | ARG | NE-CZ-NH2 | -5.63 | 117.48 | 120.30 |
| 1 | B | 56 | ASP | CB-CG-OD2 | -5.63 | 113.23 | 118.30 |
| 1 | B | 83 | ASP | CB-CG-OD2 | -5.61 | 113.26 | 118.30 |
| 1 | G | 87 | ASP | CB-CG-OD1 | -5.60 | 113.26 | 118.30 |
| 1 | G | 83 | ASP | CB-CG-OD2 | -5.58 | 113.27 | 118.30 |
| 1 | B | 98 | ASP | CB-CG-OD1 | 5.58 | 123.32 | 118.30 |
| 1 | G | 24 | ASP | CB-CG-OD2 | -5.56 | 113.30 | 118.30 |
| 1 | E | 75 | ASP | CB-CG-OD2 | -5.52 | 113.33 | 118.30 |
| 1 | C | 24 | ASP | CB-CG-OD1 | 5.51 | 123.26 | 118.30 |
| 1 | E | 117 | ARG | NE-CZ-NH1 | 5.50 | 123.05 | 120.30 |
| 1 | F | 63 | ASP | CB-CG-OD1 | 5.50 | 123.25 | 118.30 |
| 1 | H | 116 | ARG | NE-CZ-NH2 | -5.47 | 117.56 | 120.30 |
| 1 | C | 63 | ASP | CB-CG-OD2 | -5.45 | 113.39 | 118.30 |
| 1 | G | 87 | ASP | CB-CG-OD2 | 5.43 | 123.19 | 118.30 |
| 1 | E | 83 | ASP | CB-CG-OD2 | -5.43 | 113.41 | 118.30 |
| 1 | G | 8 | ASP | CB-CG-OD1 | 5.41 | 123.17 | 118.30 |
| 1 | A | 24 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 1 | A | 75 | ASP | CB-CG-OD2 | -5.40 | 113.44 | 118.30 |
| 1 | B | 63 | ASP | CB-CG-OD2 | -5.38 | 113.46 | 118.30 |
| 1 | H | 63 | ASP | CB-CG-OD1 | 5.38 | 123.14 | 118.30 |
| 1 | F | 87 | ASP | CB-CG-OD2 | 5.37 | 123.13 | 118.30 |
| 1 | C | 87 | ASP | CB-CG-OD1 | -5.35 | 113.48 | 118.30 |
| 1 | H | 24 | ASP | CB-CG-OD1 | 5.34 | 123.11 | 118.30 |
| 1 | D | 75 | ASP | CB-CG-OD1 | 5.34 | 123.11 | 118.30 |
| 1 | A | 98 | ASP | CB-CG-OD1 | 5.33 | 123.09 | 118.30 |
| 1 | F | 116 | ARG | NE-CZ-NH2 | -5.32 | 117.64 | 120.30 |
| 1 | E | 98 | ASP | CB-CG-OD1 | 5.30 | 123.07 | 118.30 |
| 1 | G | 98 | ASP | CB-CG-OD1 | 5.29 | 123.06 | 118.30 |
| 1 | C | 87 | ASP | CB-CG-OD2 | 5.28 | 123.05 | 118.30 |
| 1 | G | 63 | ASP | CB-CG-OD2 | -5.27 | 113.56 | 118.30 |
| 1 | C | 8 | ASP | CB-CG-OD1 | 5.26 | 123.03 | 118.30 |
| 1 | E | 63 | ASP | CB-CG-OD2 | -5.26 | 113.56 | 118.30 |
| 1 | F | 98 | ASP | CB-CG-OD1 | 5.26 | 123.03 | 118.30 |
| 1 | H | 63 | ASP | CB-CG-OD2 | -5.26 | 113.57 | 118.30 |
| 1 | D | 116 | ARG | NE-CZ-NH2 | -5.25 | 117.68 | 120.30 |
| 1 | A | 116 | ARG | NE-CZ-NH2 | -5.24 | 117.68 | 120.30 |
| 1 | E | 8 | ASP | CB-CG-OD1 | 5.23 | 123.01 | 118.30 |
| 1 | F | 112 | ASP | CB-CG-OD2 | -5.22 | 113.60 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | H | 116 | ARG | NE-CZ-NH1 | 5.21 | 122.91 | 120.30 |
| 1 | F | 63 | ASP | CB-CG-OD2 | -5.21 | 113.61 | 118.30 |
| 1 | H | 25 | ASP | CB-CG-OD1 | 5.21 | 122.99 | 118.30 |
| 1 | B | 24 | ASP | CB-CG-OD1 | 5.18 | 122.97 | 118.30 |
| 1 | C | 98 | ASP | CB-CG-OD1 | 5.18 | 122.96 | 118.30 |
| 1 | A | 63 | ASP | CB-CG-OD1 | 5.17 | 122.96 | 118.30 |
| 1 | A | 63 | ASP | CB-CG-OD2 | -5.15 | 113.66 | 118.30 |
| 1 | D | 83 | ASP | CB-CG-OD1 | 5.14 | 122.93 | 118.30 |
| 1 | A | 83 | ASP | CB-CG-OD1 | 5.12 | 122.91 | 118.30 |
| 1 | F | 25 | ASP | CB-CG-OD1 | 5.12 | 122.91 | 118.30 |
| 1 | G | 63 | ASP | CB-CG-OD1 | 5.12 | 122.90 | 118.30 |
| 1 | F | 75 | ASP | CB-CG-OD1 | 5.09 | 122.88 | 118.30 |
| 1 | A | 8 | ASP | CB-CG-OD1 | 5.08 | 122.87 | 118.30 |
| 1 | C | 63 | ASP | CB-CG-OD1 | 5.07 | 122.86 | 118.30 |
| 1 | D | 98 | ASP | CB-CG-OD1 | 5.07 | 122.86 | 118.30 |
| 1 | H | 8 | ASP | CB-CG-OD1 | 5.06 | 122.86 | 118.30 |
| 1 | D | 25 | ASP | CB-CG-OD1 | 5.05 | 122.85 | 118.30 |
| 1 | D | 8 | ASP | CB-CG-OD1 | 5.03 | 122.83 | 118.30 |
| 1 | C | 25 | ASP | CB-CG-OD1 | 5.02 | 122.82 | 118.30 |
| 1 | G | 83 | ASP | CB-CG-OD1 | 5.02 | 122.82 | 118.30 |
| 1 | F | 8 | ASP | CB-CG-OD1 | 5.01 | 122.81 | 118.30 |
| 1 | E | 75 | ASP | CB-CG-OD1 | 5.01 | 122.81 | 118.30 |
| 1 | B | 63 | ASP | CB-CG-OD1 | 5.01 | 122.81 | 118.30 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 978 | 0 | 954 | 96 | 0 |
| 1 | B | 978 | 0 | 954 | 87 | 0 |
| 1 | C | 978 | 0 | 954 | 93 | 0 |
| 1 | D | 978 | 0 | 954 | 91 | 0 |
| 1 | E | 978 | 0 | 954 | 88 | 0 |
| 1 | F | 978 | 0 | 954 | 95 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | G | 978 | 0 | 954 | 93 | 0 |
| 1 | H | 978 | 0 | 954 | 96 | 0 |
| All | All | 7824 | 0 | 7632 | 716 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 50.

All (716) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:21:ALA:HB1 | 1:C:22:PRO:HA | 1.47 | 0.96 |
| 1:F:21:ALA:HB1 | 1:F:22:PRO:HA | 1.47 | 0.95 |
| 1:G:21:ALA:HB1 | 1:G:22:PRO:HA | 1.48 | 0.95 |
| 1:E:85:ASN:HD22 | 1:E:85:ASN:H | 1.16 | 0.94 |
| 1:A:85:ASN:H | 1:A:85:ASN:HD22 | 1.13 | 0.94 |
| 1:H:21:ALA:HB1 | 1:H:22:PRO:HA | 1.48 | 0.94 |
| 1:D:85:ASN:HD22 | 1:D:85:ASN:H | 1.15 | 0.93 |
| 1:B:21:ALA:HB1 | 1:B:22:PRO:HA | 1.50 | 0.93 |
| 1:A:93:TRP:CZ2 | 1:A:116:ARG:HD3 | 2.03 | 0.93 |
| 1:D:45:ILE:HG13 | 1:D:70:MET:CE | 1.99 | 0.93 |
| 1:D:21:ALA:HB1 | 1:D:22:PRO:HA | 1.51 | 0.93 |
| 1:C:85:ASN:HD22 | 1:C:85:ASN:H | 1.14 | 0.92 |
| 1:H:85:ASN:H | 1:H:85:ASN:HD22 | 1.16 | 0.92 |
| 1:A:21:ALA:HB1 | 1:A:22:PRO:HA | 1.50 | 0.92 |
| 1:E:93:TRP:CZ2 | 1:E:116:ARG:HD3 | 2.05 | 0.91 |
| 1:C:45:ILE:HG13 | 1:C:70:MET:HE3 | 1.53 | 0.91 |
| 1:F:45:ILE:HG13 | 1:F:70:MET:CE | 2.01 | 0.91 |
| 1:E:21:ALA:HB1 | 1:E:22:PRO:HA | 1.50 | 0.91 |
| 1:H:45:ILE:HG13 | 1:H:70:MET:CE | 2.01 | 0.90 |
| 1:C:45:ILE:HG13 | 1:C:70:MET:CE | 2.01 | 0.90 |
| 1:B:85:ASN:H | 1:B:85:ASN:HD22 | 1.14 | 0.90 |
| 1:D:93:TRP:CZ2 | 1:D:116:ARG:HD3 | 2.07 | 0.90 |
| 1:E:45:ILE:HG13 | 1:E:70:MET:CE | 2.01 | 0.90 |
| 1:H:93:TRP:CZ2 | 1:H:116:ARG:HD3 | 2.07 | 0.89 |
| 1:F:93:TRP:CZ2 | 1:F:116:ARG:HD3 | 2.07 | 0.89 |
| 1:G:85:ASN:HD22 | 1:G:85:ASN:H | 1.14 | 0.89 |
| 1:B:93:TRP:CZ2 | 1:B:116:ARG:HD3 | 2.07 | 0.88 |
| 1:F:85:ASN:HD22 | 1:F:85:ASN:H | 1.15 | 0.88 |
| 1:C:93:TRP:CZ2 | 1:C:116:ARG:HD3 | 2.07 | 0.88 |
| 1:G:45:ILE:HG13 | 1:G:70:MET:CE | 2.03 | 0.88 |
| 1:G:93:TRP:CZ2 | 1:G:116:ARG:HD3 | 2.07 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:45:ILE:HG13 | 1:B:70:MET:CE | 2.05 | 0.86 |
| 1:C:116:ARG:HH11 | 1:C:116:ARG:HG2 | 1.41 | 0.86 |
| 1:A:45:ILE:HG13 | 1:A:70:MET:CE | 2.05 | 0.86 |
| 1:F:43:TRP:HE1 | 1:F:62:LEU:HD13 | 1.41 | 0.86 |
| 1:E:116:ARG:HG2 | 1:E:116:ARG:HH11 | 1.41 | 0.85 |
| 1:G:116:ARG:HG2 | 1:G:116:ARG:HH11 | 1.41 | 0.85 |
| 1:E:43:TRP:HE1 | 1:E:62:LEU:HD13 | 1.40 | 0.85 |
| 1:G:43:TRP:HE1 | 1:G:62:LEU:HD13 | 1.42 | 0.84 |
| 1:H:116:ARG:HH11 | 1:H:116:ARG:HG2 | 1.41 | 0.84 |
| 1:D:43:TRP:HE1 | 1:D:62:LEU:HD13 | 1.43 | 0.84 |
| 1:F:45:ILE:HG13 | 1:F:70:MET:HE1 | 1.59 | 0.84 |
| 1:D:45:ILE:CD1 | 1:D:91:ILE:HG12 | 2.08 | 0.84 |
| 1:D:116:ARG:HG2 | 1:D:116:ARG:HH11 | 1.42 | 0.84 |
| 1:C:43:TRP:HE1 | 1:C:62:LEU:HD13 | 1.43 | 0.83 |
| 1:E:45:ILE:CD1 | 1:E:91:ILE:HG12 | 2.07 | 0.83 |
| 1:A:116:ARG:HH11 | 1:A:116:ARG:HG2 | 1.42 | 0.83 |
| 1:B:116:ARG:HH11 | 1:B:116:ARG:HG2 | 1.42 | 0.83 |
| 1:A:43:TRP:HE1 | 1:A:62:LEU:HD13 | 1.41 | 0.83 |
| 1:F:116:ARG:HH11 | 1:F:116:ARG:HG2 | 1.43 | 0.83 |
| 1:H:43:TRP:HE1 | 1:H:62:LEU:HD13 | 1.42 | 0.83 |
| 1:C:45:ILE:CD1 | 1:C:91:ILE:HG12 | 2.09 | 0.83 |
| 1:B:43:TRP:HE1 | 1:B:62:LEU:HD13 | 1.43 | 0.82 |
| 1:D:45:ILE:HG13 | 1:D:70:MET:HE3 | 1.61 | 0.82 |
| 1:B:34:THR:OG1 | 1:B:67:LYS:HB3 | 1.79 | 0.82 |
| 1:H:45:ILE:CD1 | 1:H:91:ILE:HG12 | 2.09 | 0.82 |
| 1:G:34:THR:OG1 | 1:G:67:LYS:HB3 | 1.80 | 0.81 |
| 1:A:84:LEU:HB3 | 1:A:124:TYR:CD2 | 2.15 | 0.81 |
| 1:A:85:ASN:ND2 | 1:A:85:ASN:N | 2.27 | 0.81 |
| 1:G:85:ASN:ND2 | 1:G:85:ASN:N | 2.27 | 0.81 |
| 1:C:85:ASN:N | 1:C:85:ASN:ND2 | 2.28 | 0.81 |
| 1:H:97:PRO:HG3 | 1:H:108:TRP:NE1 | 1.96 | 0.81 |
| 1:F:45:ILE:CD1 | 1:F:91:ILE:HG12 | 2.11 | 0.81 |
| 1:C:34:THR:OG1 | 1:C:67:LYS:HB3 | 1.80 | 0.81 |
| 1:E:34:THR:OG1 | 1:E:67:LYS:HB3 | 1.81 | 0.81 |
| 1:A:45:ILE:CD1 | 1:A:91:ILE:HG12 | 2.11 | 0.80 |
| 1:D:85:ASN:N | 1:D:85:ASN:ND2 | 2.29 | 0.80 |
| 1:F:85:ASN:ND2 | 1:F:85:ASN:N | 2.28 | 0.80 |
| 1:F:34:THR:OG1 | 1:F:67:LYS:HB3 | 1.81 | 0.80 |
| 1:B:85:ASN:N | 1:B:85:ASN:ND2 | 2.28 | 0.80 |
| 1:E:85:ASN:N | 1:E:85:ASN:ND2 | 2.29 | 0.80 |
| 1:E:45:ILE:HG13 | 1:E:70:MET:HE3 | 1.64 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:85:ASN:N | 1:H:85:ASN:ND2 | 2.29 | 0.79 |
| 1:D:34:THR:OG1 | 1:D:67:LYS:HB3 | 1.82 | 0.79 |
| 1:H:45:ILE:HG13 | 1:H:70:MET:HE3 | 1.65 | 0.79 |
| 1:G:85:ASN:HD22 | 1:G:85:ASN:N | 1.79 | 0.79 |
| 1:G:45:ILE:CD1 | 1:G:91:ILE:HG12 | 2.11 | 0.79 |
| 1:C:85:ASN:HD22 | 1:C:85:ASN:N | 1.81 | 0.79 |
| 1:A:45:ILE:HG13 | 1:A:70:MET:HE3 | 1.63 | 0.79 |
| 1:A:85:ASN:N | 1:A:85:ASN:HD22 | 1.79 | 0.79 |
| 1:B:85:ASN:N | 1:B:85:ASN:HD22 | 1.80 | 0.79 |
| 1:H:34:THR:OG1 | 1:H:67:LYS:HB3 | 1.83 | 0.79 |
| 1:B:84:LEU:HB3 | 1:B:124:TYR:CD2 | 2.18 | 0.79 |
| 1:A:34:THR:OG1 | 1:A:67:LYS:HB3 | 1.82 | 0.79 |
| 1:E:85:ASN:HD22 | 1:E:85:ASN:N | 1.82 | 0.78 |
| 1:D:84:LEU:HB3 | 1:D:124:TYR:CD2 | 2.18 | 0.78 |
| 1:H:84:LEU:HB3 | 1:H:124:TYR:CD2 | 2.18 | 0.78 |
| 1:H:85:ASN:N | 1:H:85:ASN:HD22 | 1.81 | 0.78 |
| 1:H:45:ILE:HG13 | 1:H:70:MET:HE1 | 1.66 | 0.78 |
| 1:G:45:ILE:HG13 | 1:G:70:MET:HE1 | 1.64 | 0.78 |
| 1:B:45:ILE:CD1 | 1:B:91:ILE:HG12 | 2.15 | 0.77 |
| 1:F:84:LEU:HB3 | 1:F:124:TYR:CD2 | 2.20 | 0.77 |
| 1:B:45:ILE:HG13 | 1:B:70:MET:HE3 | 1.65 | 0.77 |
| 1:E:84:LEU:HB3 | 1:E:124:TYR:CD2 | 2.19 | 0.76 |
| 1:D:17:ILE:CG2 | 1:D:122:ILE:HD12 | 2.15 | 0.76 |
| 1:D:85:ASN:HD22 | 1:D:85:ASN:N | 1.81 | 0.76 |
| 1:F:85:ASN:HD22 | 1:F:85:ASN:N | 1.80 | 0.76 |
| 1:G:84:LEU:HB3 | 1:G:124:TYR:CD2 | 2.20 | 0.76 |
| 1:E:45:ILE:HG13 | 1:E:70:MET:HE1 | 1.66 | 0.75 |
| 1:C:84:LEU:HB3 | 1:C:124:TYR:CD2 | 2.21 | 0.75 |
| 1:F:55:VAL:HG11 | 1:F:70:MET:HE3 | 1.68 | 0.75 |
| 1:H:96:THR:HG22 | 1:H:97:PRO:HD2 | 1.68 | 0.75 |
| 1:E:17:ILE:CG2 | 1:E:122:ILE:HD12 | 2.17 | 0.75 |
| 1:D:45:ILE:HG13 | 1:D:70:MET:HE1 | 1.67 | 0.74 |
| 1:D:55:VAL:HG11 | 1:D:70:MET:CE | 2.18 | 0.74 |
| 1:H:96:THR:CB | 1:H:97:PRO:HD2 | 2.17 | 0.74 |
| 1:E:43:TRP:NE1 | 1:E:62:LEU:HD13 | 2.02 | 0.74 |
| 1:A:85:ASN:ND2 | 1:A:85:ASN:H | 1.85 | 0.74 |
| 1:E:43:TRP:HE1 | 1:E:62:LEU:CD1 | 2.01 | 0.74 |
| 1:B:17:ILE:CG2 | 1:B:122:ILE:HD12 | 2.19 | 0.73 |
| 1:F:43:TRP:HE1 | 1:F:62:LEU:CD1 | 2.01 | 0.73 |
| 1:F:55:VAL:HG11 | 1:F:70:MET:CE | 2.18 | 0.73 |
| 1:G:55:VAL:HG11 | 1:G:70:MET:HE3 | 1.69 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:43:TRP:NE1 | 1:A:62:LEU:HD13 | 2.03 | 0.73 |
| 1:C:53:LEU:HD23 | 1:C:53:LEU:N | 2.04 | 0.73 |
| 1:H:55:VAL:HG11 | 1:H:70:MET:CE | 2.19 | 0.73 |
| 1:G:43:TRP:NE1 | 1:G:62:LEU:HD13 | 2.04 | 0.72 |
| 1:F:45:ILE:HG13 | 1:F:70:MET:HE3 | 1.71 | 0.72 |
| 1:E:78:ASN:OD1 | 1:E:80:ALA:HB3 | 1.89 | 0.72 |
| 1:F:85:ASN:ND2 | 1:F:85:ASN:H | 1.86 | 0.72 |
| 1:C:43:TRP:NE1 | 1:C:62:LEU:HD13 | 2.04 | 0.72 |
| 1:H:43:TRP:NE1 | 1:H:62:LEU:HD13 | 2.03 | 0.72 |
| 1:D:43:TRP:HE1 | 1:D:62:LEU:CD1 | 2.02 | 0.72 |
| 1:F:43:TRP:NE1 | 1:F:62:LEU:HD13 | 2.03 | 0.72 |
| 1:G:55:VAL:HG11 | 1:G:70:MET:CE | 2.19 | 0.72 |
| 1:C:55:VAL:HG11 | 1:C:70:MET:CE | 2.20 | 0.72 |
| 1:G:77:PHE:HB2 | 1:G:82:GLU:OE2 | 1.88 | 0.72 |
| 1:C:43:TRP:HE1 | 1:C:62:LEU:CD1 | 2.02 | 0.72 |
| 1:C:17:ILE:CG2 | 1:C:122:ILE:HD12 | 2.20 | 0.72 |
| 1:G:85:ASN:ND2 | 1:G:85:ASN:H | 1.85 | 0.71 |
| 1:A:55:VAL:HG11 | 1:A:70:MET:CE | 2.19 | 0.71 |
| 1:D:43:TRP:NE1 | 1:D:62:LEU:HD13 | 2.04 | 0.71 |
| 1:G:43:TRP:HE1 | 1:G:62:LEU:CD1 | 2.02 | 0.71 |
| 1:G:55:VAL:HG12 | 1:G:56:ASP:H | 1.56 | 0.71 |
| 1:A:55:VAL:HG12 | 1:A:56:ASP:H | 1.56 | 0.71 |
| 1:A:43:TRP:HE1 | 1:A:62:LEU:CD1 | 2.02 | 0.71 |
| 1:A:17:ILE:CG2 | 1:A:122:ILE:HD12 | 2.21 | 0.71 |
| 1:B:45:ILE:HG13 | 1:B:70:MET:HE1 | 1.73 | 0.70 |
| 1:E:53:LEU:N | 1:E:53:LEU:HD23 | 2.04 | 0.70 |
| 1:G:45:ILE:HG13 | 1:G:70:MET:HE3 | 1.70 | 0.70 |
| 1:B:43:TRP:NE1 | 1:B:62:LEU:HD13 | 2.06 | 0.70 |
| 1:E:55:VAL:HG11 | 1:E:70:MET:CE | 2.21 | 0.70 |
| 1:B:44:ALA:HB2 | 1:B:59:SER:CB | 2.22 | 0.70 |
| 1:H:43:TRP:HE1 | 1:H:62:LEU:CD1 | 2.03 | 0.70 |
| 1:B:44:ALA:HB2 | 1:B:59:SER:HB3 | 1.74 | 0.70 |
| 1:E:44:ALA:HB2 | 1:E:59:SER:CB | 2.22 | 0.70 |
| 1:E:44:ALA:HB2 | 1:E:59:SER:HB3 | 1.74 | 0.70 |
| 1:A:53:LEU:N | 1:A:53:LEU:HD23 | 2.06 | 0.70 |
| 1:C:85:ASN:ND2 | 1:C:85:ASN:H | 1.84 | 0.69 |
| 1:H:17:ILE:CG2 | 1:H:122:ILE:HD12 | 2.22 | 0.69 |
| 1:H:55:VAL:HG12 | 1:H:56:ASP:H | 1.57 | 0.69 |
| 1:C:63:ASP:HB3 | 1:C:64:PRO:HD2 | 1.74 | 0.69 |
| 1:A:63:ASP:HB3 | 1:A:64:PRO:HD2 | 1.73 | 0.69 |
| 1:D:63:ASP:HB3 | 1:D:64:PRO:HD2 | 1.74 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:53:LEU:N | 1:D:53:LEU:HD23 | 2.07 | 0.69 |
| 1:B:55:VAL:HG12 | 1:B:56:ASP:H | 1.56 | 0.69 |
| 1:E:63:ASP:HB3 | 1:E:64:PRO:HD2 | 1.73 | 0.69 |
| 1:B:55:VAL:HG11 | 1:B:70:MET:CE | 2.22 | 0.69 |
| 1:A:44:ALA:HB2 | 1:A:59:SER:CB | 2.23 | 0.69 |
| 1:G:53:LEU:HD23 | 1:G:53:LEU:N | 2.08 | 0.69 |
| 1:B:8:ASP:O | 1:B:36:ALA:HB3 | 1.93 | 0.69 |
| 1:F:8:ASP:O | 1:F:36:ALA:HB3 | 1.93 | 0.69 |
| 1:C:119:ASN:N | 1:D:112:ASP:OD1 | 2.26 | 0.69 |
| 1:G:44:ALA:HB2 | 1:G:59:SER:CB | 2.23 | 0.68 |
| 1:A:45:ILE:HG13 | 1:A:70:MET:HE1 | 1.74 | 0.68 |
| 1:D:55:VAL:HG11 | 1:D:70:MET:HE3 | 1.74 | 0.68 |
| 1:A:44:ALA:HB2 | 1:A:59:SER:HB3 | 1.76 | 0.68 |
| 1:D:8:ASP:O | 1:D:36:ALA:HB3 | 1.93 | 0.68 |
| 1:C:55:VAL:HG12 | 1:C:56:ASP:H | 1.59 | 0.68 |
| 1:H:55:VAL:HG11 | 1:H:70:MET:HE3 | 1.75 | 0.68 |
| 1:E:55:VAL:HG12 | 1:E:56:ASP:H | 1.59 | 0.68 |
| 1:G:63:ASP:HB3 | 1:G:64:PRO:HD2 | 1.74 | 0.68 |
| 1:F:44:ALA:HB2 | 1:F:59:SER:CB | 2.24 | 0.68 |
| 1:H:63:ASP:HB3 | 1:H:64:PRO:HD2 | 1.75 | 0.68 |
| 1:B:63:ASP:HB3 | 1:B:64:PRO:HD2 | 1.75 | 0.68 |
| 1:E:57:PRO:HD2 | 1:E:70:MET:HB2 | 1.76 | 0.67 |
| 1:F:63:ASP:HB3 | 1:F:64:PRO:HD2 | 1.74 | 0.67 |
| 1:C:44:ALA:HB2 | 1:C:59:SER:HB3 | 1.75 | 0.67 |
| 1:F:44:ALA:HB2 | 1:F:59:SER:HB3 | 1.76 | 0.67 |
| 1:B:85:ASN:H | 1:B:85:ASN:ND2 | 1.86 | 0.67 |
| 1:C:44:ALA:HB2 | 1:C:59:SER:CB | 2.23 | 0.67 |
| 1:A:78:ASN:O | 1:A:80:ALA:N | 2.28 | 0.67 |
| 1:E:55:VAL:HG11 | 1:E:70:MET:HE3 | 1.75 | 0.67 |
| 1:G:44:ALA:HB2 | 1:G:59:SER:HB3 | 1.76 | 0.67 |
| 1:H:8:ASP:O | 1:H:36:ALA:HB3 | 1.94 | 0.67 |
| 1:D:55:VAL:HG12 | 1:D:56:ASP:H | 1.59 | 0.66 |
| 1:H:53:LEU:N | 1:H:53:LEU:HD23 | 2.08 | 0.66 |
| 1:A:93:TRP:CE2 | 1:A:116:ARG:HD3 | 2.30 | 0.66 |
| 1:B:43:TRP:HE1 | 1:B:62:LEU:CD1 | 2.07 | 0.66 |
| 1:G:8:ASP:O | 1:G:36:ALA:HB3 | 1.95 | 0.66 |
| 1:D:44:ALA:HB2 | 1:D:59:SER:HB3 | 1.76 | 0.66 |
| 1:D:44:ALA:HB2 | 1:D:59:SER:CB | 2.26 | 0.66 |
| 1:C:55:VAL:HG11 | 1:C:70:MET:HE2 | 1.78 | 0.66 |
| 1:D:63:ASP:HB3 | 1:D:64:PRO:CD | 2.26 | 0.66 |
| 1:H:96:THR:CG2 | 1:H:97:PRO:HD2 | 2.25 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:53:LEU:N | 1:B:53:LEU:HD23 | 2.09 | 0.66 |
| 1:H:44:ALA:HB2 | 1:H:59:SER:CB | 2.26 | 0.65 |
| 1:F:55:VAL:HG12 | 1:F:56:ASP:H | 1.59 | 0.65 |
| 1:H:55:VAL:HG12 | 1:H:56:ASP:N | 2.11 | 0.65 |
| 1:A:63:ASP:HB3 | 1:A:64:PRO:CD | 2.26 | 0.65 |
| 1:F:53:LEU:N | 1:F:53:LEU:HD23 | 2.09 | 0.65 |
| 1:E:93:TRP:CE2 | 1:E:116:ARG:HD3 | 2.31 | 0.65 |
| 1:B:17:ILE:HG22 | 1:B:122:ILE:HD12 | 1.77 | 0.65 |
| 1:C:8:ASP:O | 1:C:36:ALA:HB3 | 1.97 | 0.65 |
| 1:F:17:ILE:CG2 | 1:F:122:ILE:HD12 | 2.26 | 0.65 |
| 1:B:55:VAL:HG12 | 1:B:56:ASP:N | 2.12 | 0.65 |
| 1:H:44:ALA:HB2 | 1:H:59:SER:HB3 | 1.78 | 0.65 |
| 1:G:55:VAL:HG12 | 1:G:56:ASP:N | 2.11 | 0.65 |
| 1:C:55:VAL:HG12 | 1:C:56:ASP:N | 2.12 | 0.65 |
| 1:A:55:VAL:HG11 | 1:A:70:MET:HE3 | 1.77 | 0.65 |
| 1:E:63:ASP:HB3 | 1:E:64:PRO:CD | 2.26 | 0.65 |
| 1:H:63:ASP:HB3 | 1:H:64:PRO:CD | 2.27 | 0.65 |
| 1:A:96:THR:HG22 | 1:A:97:PRO:HD2 | 1.79 | 0.65 |
| 1:H:97:PRO:HG3 | 1:H:108:TRP:CD1 | 2.31 | 0.65 |
| 1:E:31:ILE:HG22 | 1:E:32:LYS:N | 2.12 | 0.65 |
| 1:A:55:VAL:HG12 | 1:A:56:ASP:N | 2.12 | 0.64 |
| 1:C:78:ASN:O | 1:C:80:ALA:N | 2.31 | 0.64 |
| 1:H:57:PRO:HD2 | 1:H:70:MET:HB2 | 1.80 | 0.64 |
| 1:B:57:PRO:HD2 | 1:B:70:MET:HB2 | 1.79 | 0.64 |
| 1:D:57:PRO:HD2 | 1:D:70:MET:HB2 | 1.78 | 0.64 |
| 1:F:55:VAL:HG12 | 1:F:56:ASP:N | 2.13 | 0.64 |
| 1:E:8:ASP:O | 1:E:36:ALA:HB3 | 1.97 | 0.64 |
| 1:C:63:ASP:HB3 | 1:C:64:PRO:CD | 2.28 | 0.64 |
| 1:G:63:ASP:HB3 | 1:G:64:PRO:CD | 2.27 | 0.64 |
| 1:B:63:ASP:HB3 | 1:B:64:PRO:CD | 2.28 | 0.64 |
| 1:D:31:ILE:HG22 | 1:D:32:LYS:N | 2.13 | 0.64 |
| 1:C:17:ILE:HG22 | 1:C:122:ILE:HD12 | 1.78 | 0.64 |
| 1:F:5:PRO:HA | 1:F:114:MET:HE3 | 1.79 | 0.64 |
| 1:C:31:ILE:HG22 | 1:C:32:LYS:N | 2.13 | 0.63 |
| 1:F:57:PRO:HD2 | 1:F:70:MET:HB2 | 1.79 | 0.63 |
| 1:A:68:VAL:HG22 | 1:A:69:LEU:N | 2.14 | 0.63 |
| 1:D:17:ILE:HG22 | 1:D:122:ILE:HD12 | 1.78 | 0.63 |
| 1:E:17:ILE:HG22 | 1:E:122:ILE:HD12 | 1.80 | 0.63 |
| 1:C:45:ILE:HG13 | 1:C:70:MET:HE1 | 1.79 | 0.63 |
| 1:H:5:PRO:HA | 1:H:114:MET:HE3 | 1.81 | 0.63 |
| 1:F:63:ASP:HB3 | 1:F:64:PRO:CD | 2.28 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:68:VAL:HG22 | 1:D:69:LEU:N | 2.14 | 0.63 |
| 1:D:78:ASN:OD1 | 1:D:80:ALA:HB3 | 1.99 | 0.62 |
| 1:A:57:PRO:HD2 | 1:A:70:MET:HB2 | 1.80 | 0.62 |
| 1:H:31:ILE:HG22 | 1:H:32:LYS:N | 2.14 | 0.62 |
| 1:A:25:ASP:CG | 1:E:40:ARG:HH22 | 2.01 | 0.62 |
| 1:D:93:TRP:CE2 | 1:D:116:ARG:HD3 | 2.34 | 0.62 |
| 1:E:55:VAL:HG12 | 1:E:56:ASP:N | 2.14 | 0.62 |
| 1:A:17:ILE:HG22 | 1:A:122:ILE:HD12 | 1.81 | 0.62 |
| 1:C:93:TRP:CE2 | 1:C:116:ARG:HD3 | 2.33 | 0.62 |
| 1:B:78:ASN:OD1 | 1:B:80:ALA:HB3 | 2.00 | 0.62 |
| 1:B:31:ILE:HG22 | 1:B:32:LYS:N | 2.14 | 0.62 |
| 1:C:5:PRO:HG2 | 1:G:80:ALA:O | 2.00 | 0.62 |
| 1:G:93:TRP:CE2 | 1:G:116:ARG:HD3 | 2.34 | 0.62 |
| 1:H:78:ASN:O | 1:H:80:ALA:N | 2.33 | 0.61 |
| 1:C:57:PRO:HD2 | 1:C:70:MET:HB2 | 1.80 | 0.61 |
| 1:G:57:PRO:HD2 | 1:G:70:MET:HB2 | 1.80 | 0.61 |
| 1:B:68:VAL:HG22 | 1:B:69:LEU:N | 2.15 | 0.61 |
| 1:B:96:THR:HG22 | 1:B:97:PRO:HD2 | 1.82 | 0.61 |
| 1:H:93:TRP:CE2 | 1:H:116:ARG:HD3 | 2.35 | 0.61 |
| 1:B:93:TRP:CE2 | 1:B:116:ARG:HD3 | 2.35 | 0.61 |
| 1:B:55:VAL:HG11 | 1:B:70:MET:HE3 | 1.81 | 0.61 |
| 1:D:55:VAL:HG12 | 1:D:56:ASP:N | 2.15 | 0.61 |
| 1:G:5:PRO:HA | 1:G:114:MET:HE3 | 1.81 | 0.61 |
| 1:D:5:PRO:HG3 | 1:G:81:THR:CG2 | 2.30 | 0.61 |
| 1:H:81:THR:O | 1:H:82:GLU:HG2 | 1.99 | 0.61 |
| 1:H:97:PRO:HG3 | 1:H:108:TRP:HE1 | 1.65 | 0.61 |
| 1:D:45:ILE:HD11 | 1:D:91:ILE:HG12 | 1.82 | 0.61 |
| 1:F:93:TRP:CE2 | 1:F:116:ARG:HD3 | 2.35 | 0.60 |
| 1:F:31:ILE:HG22 | 1:F:32:LYS:N | 2.16 | 0.60 |
| 1:A:8:ASP:O | 1:A:36:ALA:HB3 | 2.01 | 0.60 |
| 1:G:116:ARG:CG | 1:G:116:ARG:HH11 | 2.14 | 0.60 |
| 1:C:45:ILE:HD11 | 1:C:91:ILE:HG12 | 1.84 | 0.60 |
| 1:C:116:ARG:HH11 | 1:C:116:ARG:CG | 2.14 | 0.60 |
| 1:F:109:PHE:O | 1:G:117:ARG:NH1 | 2.33 | 0.60 |
| 1:G:17:ILE:CG2 | 1:G:122:ILE:HD12 | 2.32 | 0.60 |
| 1:E:68:VAL:HG22 | 1:E:69:LEU:N | 2.17 | 0.59 |
| 1:F:68:VAL:HG22 | 1:F:69:LEU:N | 2.16 | 0.59 |
| 1:B:18:VAL:HG13 | 1:B:123:GLU:O | 2.03 | 0.59 |
| 1:A:25:ASP:OD1 | 1:E:40:ARG:NH2 | 2.31 | 0.59 |
| 1:A:78:ASN:OD1 | 1:A:80:ALA:HB3 | 2.02 | 0.59 |
| 1:D:116:ARG:CG | 1:D:116:ARG:HH11 | 2.14 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:22:PRO:HB3 | 1:C:12:GLN:OE1 | 2.03 | 0.59 |
| 1:A:84:LEU:HB3 | 1:A:124:TYR:HD2 | 1.66 | 0.59 |
| 1:H:78:ASN:OD1 | 1:H:80:ALA:HB3 | 2.02 | 0.59 |
| 1:C:68:VAL:HG22 | 1:C:69:LEU:N | 2.17 | 0.59 |
| 1:F:116:ARG:HH11 | 1:F:116:ARG:CG | 2.15 | 0.58 |
| 1:G:31:ILE:HG22 | 1:G:32:LYS:N | 2.18 | 0.58 |
| 1:F:81:THR:O | 1:F:82:GLU:HG2 | 2.02 | 0.58 |
| 1:E:45:ILE:HD11 | 1:E:91:ILE:HG12 | 1.83 | 0.58 |
| 1:H:68:VAL:HG22 | 1:H:69:LEU:N | 2.18 | 0.58 |
| 1:G:68:VAL:HG22 | 1:G:69:LEU:N | 2.18 | 0.58 |
| 1:A:31:ILE:HG22 | 1:A:32:LYS:N | 2.18 | 0.58 |
| 1:C:112:ASP:OD1 | 1:D:118:LYS:HA | 2.04 | 0.58 |
| 1:H:45:ILE:HD11 | 1:H:91:ILE:HG12 | 1.86 | 0.58 |
| 1:G:35:ASN:ND2 | 1:G:63:ASP:O | 2.37 | 0.57 |
| 1:B:116:ARG:HH11 | 1:B:116:ARG:CG | 2.16 | 0.57 |
| 1:E:22:PRO:HB3 | 1:F:12:GLN:OE1 | 2.04 | 0.57 |
| 1:H:116:ARG:HH11 | 1:H:116:ARG:CG | 2.16 | 0.57 |
| 1:D:55:VAL:HG11 | 1:D:70:MET:HE2 | 1.86 | 0.57 |
| 1:C:55:VAL:HG11 | 1:C:70:MET:HE3 | 1.86 | 0.57 |
| 1:A:92:GLU:HG3 | 1:A:117:ARG:HG2 | 1.86 | 0.57 |
| 1:E:116:ARG:CG | 1:E:116:ARG:HH11 | 2.14 | 0.57 |
| 1:H:17:ILE:HG22 | 1:H:122:ILE:HD12 | 1.85 | 0.57 |
| 1:A:116:ARG:HH11 | 1:A:116:ARG:CG | 2.15 | 0.56 |
| 1:C:109:PHE:O | 1:D:117:ARG:NH1 | 2.38 | 0.56 |
| 1:E:85:ASN:H | 1:E:85:ASN:ND2 | 1.87 | 0.56 |
| 1:A:35:ASN:ND2 | 1:A:63:ASP:O | 2.38 | 0.56 |
| 1:A:55:VAL:HG11 | 1:A:70:MET:HE2 | 1.86 | 0.56 |
| 1:B:55:VAL:HG11 | 1:B:70:MET:HE2 | 1.88 | 0.56 |
| 1:E:43:TRP:HA | 1:E:92:GLU:O | 2.06 | 0.56 |
| 1:G:22:PRO:HB3 | 1:H:12:GLN:OE1 | 2.06 | 0.56 |
| 1:E:96:THR:HG22 | 1:E:97:PRO:HD2 | 1.87 | 0.56 |
| 1:C:104:PHE:HA | 1:C:108:TRP:CZ3 | 2.41 | 0.56 |
| 1:H:20:ASN:HA | 1:H:125:ASN:HB3 | 1.87 | 0.56 |
| 1:C:89:ILE:N | 1:C:120:LEU:O | 2.38 | 0.55 |
| 1:F:84:LEU:HB3 | 1:F:124:TYR:HD2 | 1.70 | 0.55 |
| 1:A:104:PHE:HA | 1:A:108:TRP:CZ3 | 2.41 | 0.55 |
| 1:F:112:ASP:OD1 | 1:G:119:ASN:ND2 | 2.39 | 0.55 |
| 1:B:19:PHE:HE2 | 1:B:74:CYS:HB2 | 1.72 | 0.55 |
| 1:E:35:ASN:ND2 | 1:E:63:ASP:O | 2.39 | 0.55 |
| 1:B:84:LEU:HB3 | 1:B:124:TYR:HD2 | 1.70 | 0.55 |
| 1:C:35:ASN:ND2 | 1:C:63:ASP:O | 2.40 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:55:VAL:HG11 | 1:H:70:MET:HE2 | 1.88 | 0.55 |
| 1:F:104:PHE:HA | 1:F:108:TRP:CZ3 | 2.42 | 0.55 |
| 1:D:85:ASN:H | 1:D:85:ASN:ND2 | 1.85 | 0.55 |
| 1:F:112:ASP:OD1 | 1:G:119:ASN:N | 2.40 | 0.55 |
| 1:H:61:VAL:O | 1:H:62:LEU:HD12 | 2.07 | 0.54 |
| 1:B:35:ASN:ND2 | 1:B:63:ASP:O | 2.39 | 0.54 |
| 1:D:104:PHE:HA | 1:D:108:TRP:CZ3 | 2.43 | 0.54 |
| 1:F:89:ILE:N | 1:F:120:LEU:O | 2.39 | 0.54 |
| 1:D:5:PRO:HG3 | 1:G:81:THR:HG21 | 1.90 | 0.54 |
| 1:G:89:ILE:N | 1:G:120:LEU:O | 2.40 | 0.54 |
| 1:F:10:ASN:HB2 | 1:F:34:THR:HG22 | 1.90 | 0.54 |
| 1:D:84:LEU:HB3 | 1:D:124:TYR:HD2 | 1.73 | 0.54 |
| 1:E:84:LEU:HB3 | 1:E:124:TYR:HD2 | 1.72 | 0.53 |
| 1:H:104:PHE:HA | 1:H:108:TRP:CZ3 | 2.43 | 0.53 |
| 1:D:10:ASN:HB2 | 1:D:34:THR:HG22 | 1.90 | 0.53 |
| 1:G:84:LEU:HB3 | 1:G:124:TYR:HD2 | 1.71 | 0.53 |
| 1:A:17:ILE:CD1 | 1:A:19:PHE:CE1 | 2.92 | 0.53 |
| 1:F:17:ILE:HG22 | 1:F:122:ILE:HD12 | 1.90 | 0.53 |
| 1:B:78:ASN:O | 1:B:80:ALA:N | 2.42 | 0.53 |
| 1:A:45:ILE:HD11 | 1:A:91:ILE:HG12 | 1.89 | 0.53 |
| 1:C:18:VAL:HG12 | 1:C:19:PHE:N | 2.24 | 0.53 |
| 1:G:17:ILE:CD1 | 1:G:19:PHE:CE1 | 2.92 | 0.53 |
| 1:G:19:PHE:HE2 | 1:G:74:CYS:HB2 | 1.74 | 0.53 |
| 1:G:104:PHE:HA | 1:G:108:TRP:CZ3 | 2.44 | 0.53 |
| 1:F:78:ASN:O | 1:F:80:ALA:N | 2.42 | 0.53 |
| 1:C:92:GLU:HG3 | 1:C:117:ARG:HG2 | 1.90 | 0.53 |
| 1:B:17:ILE:CD1 | 1:B:19:PHE:CE1 | 2.92 | 0.53 |
| 1:F:5:PRO:N | 1:F:114:MET:HE1 | 2.24 | 0.53 |
| 1:D:96:THR:HG22 | 1:D:97:PRO:HD2 | 1.90 | 0.53 |
| 1:E:61:VAL:O | 1:E:62:LEU:HD12 | 2.09 | 0.52 |
| 1:C:17:ILE:CD1 | 1:C:19:PHE:CE1 | 2.92 | 0.52 |
| 1:D:35:ASN:ND2 | 1:D:63:ASP:O | 2.42 | 0.52 |
| 1:A:17:ILE:HD12 | 1:A:19:PHE:CE1 | 2.44 | 0.52 |
| 1:A:104:PHE:HA | 1:A:108:TRP:HZ3 | 1.74 | 0.52 |
| 1:E:89:ILE:N | 1:E:120:LEU:O | 2.40 | 0.52 |
| 1:C:96:THR:HG22 | 1:C:97:PRO:HD2 | 1.92 | 0.52 |
| 1:A:44:ALA:CB | 1:A:59:SER:HB3 | 2.39 | 0.52 |
| 1:F:18:VAL:HG12 | 1:F:19:PHE:N | 2.23 | 0.52 |
| 1:H:84:LEU:HB3 | 1:H:124:TYR:HD2 | 1.69 | 0.52 |
| 1:B:104:PHE:HA | 1:B:108:TRP:CZ3 | 2.44 | 0.52 |
| 1:B:10:ASN:HB2 | 1:B:34:THR:HG22 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:44:ALA:CB | 1:C:59:SER:HB3 | 2.40 | 0.52 |
| 1:F:20:ASN:HA | 1:F:125:ASN:HB3 | 1.91 | 0.52 |
| 1:A:61:VAL:O | 1:A:62:LEU:HD12 | 2.09 | 0.52 |
| 1:E:10:ASN:HB2 | 1:E:34:THR:HG22 | 1.92 | 0.52 |
| 1:C:19:PHE:HE2 | 1:C:74:CYS:HB2 | 1.74 | 0.52 |
| 1:C:28:THR:O | 1:C:28:THR:HG22 | 2.10 | 0.52 |
| 1:C:55:VAL:CG1 | 1:C:70:MET:HE2 | 2.40 | 0.52 |
| 1:F:61:VAL:O | 1:F:62:LEU:HD12 | 2.10 | 0.52 |
| 1:G:44:ALA:CB | 1:G:59:SER:HB3 | 2.40 | 0.52 |
| 1:F:17:ILE:CD1 | 1:F:19:PHE:CE1 | 2.93 | 0.52 |
| 1:C:112:ASP:OD1 | 1:D:119:ASN:N | 2.43 | 0.52 |
| 1:A:28:THR:HG22 | 1:A:28:THR:O | 2.09 | 0.52 |
| 1:A:112:ASP:HB3 | 1:B:118:LYS:HA | 1.91 | 0.52 |
| 1:E:17:ILE:CD1 | 1:E:19:PHE:CE1 | 2.93 | 0.51 |
| 1:E:18:VAL:HG13 | 1:E:123:GLU:O | 2.09 | 0.51 |
| 1:H:17:ILE:CD1 | 1:H:19:PHE:CE1 | 2.94 | 0.51 |
| 1:F:35:ASN:ND2 | 1:F:63:ASP:O | 2.43 | 0.51 |
| 1:C:104:PHE:HA | 1:C:108:TRP:HZ3 | 1.73 | 0.51 |
| 1:A:55:VAL:CG1 | 1:A:70:MET:HG3 | 2.40 | 0.51 |
| 1:H:10:ASN:HB2 | 1:H:34:THR:HG22 | 1.93 | 0.51 |
| 1:E:104:PHE:HA | 1:E:108:TRP:CZ3 | 2.45 | 0.51 |
| 1:F:21:ALA:HB1 | 1:F:22:PRO:CA | 2.32 | 0.51 |
| 1:G:45:ILE:HD11 | 1:G:91:ILE:HG12 | 1.90 | 0.51 |
| 1:D:17:ILE:CD1 | 1:D:19:PHE:CE1 | 2.93 | 0.51 |
| 1:F:44:ALA:CB | 1:F:59:SER:HB3 | 2.40 | 0.51 |
| 1:B:44:ALA:CB | 1:B:59:SER:HB3 | 2.38 | 0.51 |
| 1:H:19:PHE:HE2 | 1:H:74:CYS:HB2 | 1.75 | 0.51 |
| 1:F:45:ILE:HD11 | 1:F:91:ILE:HG12 | 1.89 | 0.51 |
| 1:E:55:VAL:HG11 | 1:E:70:MET:HE2 | 1.90 | 0.51 |
| 1:H:35:ASN:ND2 | 1:H:63:ASP:O | 2.43 | 0.51 |
| 1:B:45:ILE:HD11 | 1:B:91:ILE:HG12 | 1.92 | 0.51 |
| 1:H:89:ILE:N | 1:H:120:LEU:O | 2.43 | 0.51 |
| 1:D:61:VAL:O | 1:D:62:LEU:HD12 | 2.10 | 0.51 |
| 1:F:104:PHE:HA | 1:F:108:TRP:HZ3 | 1.75 | 0.51 |
| 1:C:55:VAL:CG1 | 1:C:70:MET:HG3 | 2.40 | 0.50 |
| 1:B:89:ILE:N | 1:B:120:LEU:O | 2.44 | 0.50 |
| 1:D:43:TRP:HA | 1:D:92:GLU:O | 2.12 | 0.50 |
| 1:A:10:ASN:HB2 | 1:A:34:THR:HG22 | 1.92 | 0.50 |
| 1:C:27:HIS:HD2 | 1:C:29:TYR:CE1 | 2.30 | 0.50 |
| 1:D:44:ALA:CB | 1:D:59:SER:HB3 | 2.41 | 0.50 |
| 1:G:5:PRO:N | 1:G:114:MET:HE1 | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:17:ILE:HG22 | 1:G:122:ILE:HD12 | 1.92 | 0.50 |
| 1:F:55:VAL:CG1 | 1:F:70:MET:HG3 | 2.40 | 0.50 |
| 1:E:18:VAL:HG12 | 1:E:19:PHE:N | 2.25 | 0.50 |
| 1:A:19:PHE:HE2 | 1:A:74:CYS:HB2 | 1.76 | 0.50 |
| 1:F:17:ILE:HD12 | 1:F:19:PHE:CE1 | 2.46 | 0.50 |
| 1:G:18:VAL:HG12 | 1:G:19:PHE:N | 2.27 | 0.50 |
| 1:A:48:THR:HG22 | 1:A:48:THR:O | 2.12 | 0.50 |
| 1:B:27:HIS:HD2 | 1:B:29:TYR:CE1 | 2.29 | 0.50 |
| 1:E:44:ALA:CB | 1:E:59:SER:HB3 | 2.39 | 0.50 |
| 1:G:55:VAL:CG1 | 1:G:70:MET:HG3 | 2.40 | 0.50 |
| 1:E:19:PHE:HE2 | 1:E:74:CYS:HB2 | 1.76 | 0.50 |
| 1:B:19:PHE:CE2 | 1:B:74:CYS:HB2 | 2.46 | 0.50 |
| 1:B:104:PHE:HA | 1:B:108:TRP:HZ3 | 1.77 | 0.50 |
| 1:G:104:PHE:HA | 1:G:108:TRP:HZ3 | 1.77 | 0.50 |
| 1:F:119:ASN:N | 1:G:112:ASP:OD1 | 2.44 | 0.50 |
| 1:A:119:ASN:N | 1:B:112:ASP:OD1 | 2.43 | 0.50 |
| 1:D:19:PHE:HE2 | 1:D:74:CYS:HB2 | 1.76 | 0.49 |
| 1:B:17:ILE:HD12 | 1:B:19:PHE:CE1 | 2.47 | 0.49 |
| 1:E:52:ARG:C | 1:E:53:LEU:HD23 | 2.32 | 0.49 |
| 1:D:89:ILE:N | 1:D:120:LEU:O | 2.43 | 0.49 |
| 1:G:55:VAL:HG11 | 1:G:70:MET:HE2 | 1.93 | 0.49 |
| 1:F:28:THR:O | 1:F:28:THR:HG22 | 2.11 | 0.49 |
| 1:E:48:THR:HG22 | 1:E:48:THR:O | 2.12 | 0.49 |
| 1:D:55:VAL:CG1 | 1:D:70:MET:HG3 | 2.43 | 0.49 |
| 1:E:92:GLU:OE2 | 1:E:117:ARG:NH2 | 2.41 | 0.49 |
| 1:F:96:THR:HG22 | 1:F:97:PRO:HD2 | 1.93 | 0.49 |
| 1:H:104:PHE:HA | 1:H:108:TRP:HZ3 | 1.77 | 0.49 |
| 1:C:84:LEU:HB3 | 1:C:124:TYR:HD2 | 1.74 | 0.49 |
| 1:C:52:ARG:C | 1:C:53:LEU:HD23 | 2.33 | 0.49 |
| 1:C:5:PRO:HA | 1:C:114:MET:HE3 | 1.95 | 0.49 |
| 1:D:104:PHE:HA | 1:D:108:TRP:HZ3 | 1.76 | 0.49 |
| 1:F:19:PHE:HE2 | 1:F:74:CYS:HB2 | 1.77 | 0.49 |
| 1:C:43:TRP:HA | 1:C:92:GLU:O | 2.13 | 0.49 |
| 1:D:18:VAL:HG12 | 1:D:19:PHE:N | 2.27 | 0.49 |
| 1:G:27:HIS:HD2 | 1:G:29:TYR:CE1 | 2.30 | 0.49 |
| 1:D:101:ALA:O | 1:D:103:GLN:N | 2.46 | 0.49 |
| 1:H:55:VAL:CG1 | 1:H:70:MET:HG3 | 2.43 | 0.49 |
| 1:G:48:THR:O | 1:G:48:THR:HG22 | 2.12 | 0.49 |
| 1:G:19:PHE:CE2 | 1:G:74:CYS:HB2 | 2.48 | 0.49 |
| 1:E:28:THR:HG22 | 1:E:28:THR:O | 2.12 | 0.49 |
| 1:B:55:VAL:CG1 | 1:B:70:MET:HG3 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:H:18:VAL:HG12 | 1:H:19:PHE:N | 2.28 | 0.48 |
| 1:B:28:THR:HG22 | 1:B:28:THR:O | 2.12 | 0.48 |
| 1:B:18:VAL:HG12 | 1:B:19:PHE:N | 2.27 | 0.48 |
| 1:F:27:HIS:HD2 | 1:F:29:TYR:CE1 | 2.31 | 0.48 |
| 1:D:28:THR:HG22 | 1:D:28:THR:O | 2.14 | 0.48 |
| 1:D:17:ILE:HD12 | 1:D:19:PHE:CE1 | 2.48 | 0.48 |
| 1:F:18:VAL:HG13 | 1:F:123:GLU:O | 2.14 | 0.48 |
| 1:E:104:PHE:HA | 1:E:108:TRP:HZ3 | 1.79 | 0.48 |
| 1:D:45:ILE:HA | 1:D:90:CYS:O | 2.13 | 0.48 |
| 1:G:61:VAL:O | 1:G:62:LEU:HD12 | 2.13 | 0.48 |
| 1:H:19:PHE:CD2 | 1:H:29:TYR:CE1 | 3.02 | 0.48 |
| 1:D:19:PHE:CE2 | 1:D:74:CYS:HB2 | 2.49 | 0.48 |
| 1:C:21:ALA:HB1 | 1:C:22:PRO:CA | 2.33 | 0.48 |
| 1:E:55:VAL:CG1 | 1:E:70:MET:HG3 | 2.43 | 0.48 |
| 1:C:19:PHE:CE2 | 1:C:74:CYS:HB2 | 2.48 | 0.48 |
| 1:A:52:ARG:C | 1:A:53:LEU:HD23 | 2.34 | 0.48 |
| 1:B:55:VAL:CG1 | 1:B:56:ASP:H | 2.27 | 0.48 |
| 1:C:10:ASN:HB2 | 1:C:34:THR:HG22 | 1.95 | 0.48 |
| 1:F:52:ARG:C | 1:F:53:LEU:HD23 | 2.35 | 0.48 |
| 1:D:46:LYS:O | 1:D:90:CYS:N | 2.39 | 0.48 |
| 1:C:17:ILE:HD12 | 1:C:19:PHE:CE1 | 2.49 | 0.48 |
| 1:F:19:PHE:CE2 | 1:F:74:CYS:HB2 | 2.49 | 0.48 |
| 1:G:78:ASN:O | 1:G:80:ALA:N | 2.46 | 0.48 |
| 1:G:28:THR:O | 1:G:28:THR:HG22 | 2.14 | 0.48 |
| 1:H:48:THR:HG22 | 1:H:48:THR:O | 2.13 | 0.48 |
| 1:E:45:ILE:HA | 1:E:90:CYS:O | 2.14 | 0.47 |
| 1:E:92:GLU:OE2 | 1:E:117:ARG:NE | 2.47 | 0.47 |
| 1:G:10:ASN:HB2 | 1:G:34:THR:HG22 | 1.95 | 0.47 |
| 1:H:97:PRO:CG | 1:H:108:TRP:NE1 | 2.73 | 0.47 |
| 1:H:44:ALA:CB | 1:H:59:SER:HB3 | 2.44 | 0.47 |
| 1:B:94:THR:OG1 | 1:B:95:ASN:N | 2.46 | 0.47 |
| 1:D:20:ASN:HA | 1:D:125:ASN:HB3 | 1.95 | 0.47 |
| 1:E:19:PHE:CE2 | 1:E:74:CYS:HB2 | 2.49 | 0.47 |
| 1:F:118:LYS:HA | 1:G:112:ASP:OD1 | 2.14 | 0.47 |
| 1:F:40:ARG:HB3 | 1:F:96:THR:OG1 | 2.15 | 0.47 |
| 1:F:48:THR:O | 1:F:48:THR:HG22 | 2.14 | 0.47 |
| 1:D:43:TRP:CD1 | 1:D:62:LEU:HD13 | 2.49 | 0.47 |
| 1:C:61:VAL:O | 1:C:62:LEU:HD12 | 2.13 | 0.47 |
| 1:H:17:ILE:HD12 | 1:H:19:PHE:CE1 | 2.49 | 0.47 |
| 1:D:27:HIS:HD2 | 1:D:29:TYR:CE1 | 2.33 | 0.47 |
| 1:E:17:ILE:HD12 | 1:E:19:PHE:CE1 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:H:19:PHE:CE2 | 1:H:74:CYS:HB2 | 2.49 | 0.47 |
| 1:D:68:VAL:HG22 | 1:D:69:LEU:H | 1.78 | 0.47 |
| 1:H:43:TRP:CD1 | 1:H:62:LEU:HD13 | 2.50 | 0.47 |
| 1:A:27:HIS:HD2 | 1:A:29:TYR:CE1 | 2.32 | 0.47 |
| 1:A:68:VAL:CG2 | 1:A:69:LEU:N | 2.78 | 0.47 |
| 1:G:105:ARG:N | 1:G:108:TRP:CZ3 | 2.79 | 0.47 |
| 1:G:12:GLN:OE1 | 1:H:22:PRO:HB3 | 2.15 | 0.47 |
| 1:F:5:PRO:N | 1:F:114:MET:CE | 2.78 | 0.47 |
| 1:A:109:PHE:O | 1:B:117:ARG:NH1 | 2.48 | 0.47 |
| 1:F:43:TRP:CD1 | 1:F:62:LEU:HD13 | 2.50 | 0.47 |
| 1:H:55:VAL:CG1 | 1:H:56:ASP:H | 2.27 | 0.47 |
| 1:E:43:TRP:CD1 | 1:E:62:LEU:HD13 | 2.50 | 0.47 |
| 1:B:61:VAL:O | 1:B:62:LEU:HD12 | 2.15 | 0.47 |
| 1:H:27:HIS:HD2 | 1:H:29:TYR:CE1 | 2.33 | 0.47 |
| 1:D:68:VAL:CG2 | 1:D:69:LEU:N | 2.77 | 0.47 |
| 1:A:19:PHE:CE2 | 1:A:74:CYS:HB2 | 2.50 | 0.46 |
| 1:A:68:VAL:HG22 | 1:A:69:LEU:H | 1.80 | 0.46 |
| 1:A:101:ALA:O | 1:A:103:GLN:N | 2.48 | 0.46 |
| 1:G:55:VAL:CG1 | 1:G:56:ASP:N | 2.78 | 0.46 |
| 1:A:18:VAL:HG12 | 1:A:19:PHE:N | 2.29 | 0.46 |
| 1:G:17:ILE:HD12 | 1:G:19:PHE:CE1 | 2.50 | 0.46 |
| 1:C:48:THR:O | 1:C:48:THR:HG22 | 2.14 | 0.46 |
| 1:H:28:THR:O | 1:H:28:THR:HG22 | 2.15 | 0.46 |
| 1:A:89:ILE:N | 1:A:120:LEU:O | 2.48 | 0.46 |
| 1:F:55:VAL:HG11 | 1:F:70:MET:HE2 | 1.94 | 0.46 |
| 1:A:43:TRP:CD1 | 1:A:62:LEU:HD13 | 2.50 | 0.46 |
| 1:D:19:PHE:CD2 | 1:D:29:TYR:CE1 | 3.03 | 0.46 |
| 1:D:31:ILE:CG2 | 1:D:32:LYS:N | 2.78 | 0.46 |
| 1:D:120:LEU:HD23 | 1:D:120:LEU:HA | 1.54 | 0.46 |
| 1:E:46:LYS:O | 1:E:90:CYS:N | 2.41 | 0.46 |
| 1:D:52:ARG:C | 1:D:53:LEU:HD23 | 2.36 | 0.46 |
| 1:A:97:PRO:HG2 | 1:A:108:TRP:HE1 | 1.81 | 0.46 |
| 1:B:97:PRO:CG | 1:B:108:TRP:NE1 | 2.79 | 0.46 |
| 1:G:55:VAL:CG1 | 1:G:56:ASP:H | 2.26 | 0.46 |
| 1:E:27:HIS:HD2 | 1:E:29:TYR:CE1 | 2.33 | 0.46 |
| 1:G:52:ARG:C | 1:G:53:LEU:HD23 | 2.36 | 0.46 |
| 1:F:19:PHE:CD2 | 1:F:29:TYR:CE1 | 3.04 | 0.46 |
| 1:D:40:ARG:HB3 | 1:D:96:THR:OG1 | 2.16 | 0.46 |
| 1:A:55:VAL:CG1 | 1:A:56:ASP:H | 2.26 | 0.46 |
| 1:G:43:TRP:CD1 | 1:G:62:LEU:HD13 | 2.51 | 0.46 |
| 1:C:122:ILE:CD1 | 1:C:122:ILE:N | 2.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:5:PRO:CA | 1:F:114:MET:HE3 | 2.45 | 0.46 |
| 1:A:105:ARG:N | 1:A:108:TRP:CZ3 | 2.77 | 0.46 |
| 1:G:19:PHE:CD2 | 1:G:29:TYR:CE1 | 3.04 | 0.46 |
| 1:A:120:LEU:HD23 | 1:A:120:LEU:HA | 1.51 | 0.46 |
| 1:F:21:ALA:CB | 1:F:22:PRO:HA | 2.28 | 0.45 |
| 1:B:55:VAL:CG1 | 1:B:56:ASP:N | 2.79 | 0.45 |
| 1:C:43:TRP:CD1 | 1:C:62:LEU:HD13 | 2.50 | 0.45 |
| 1:D:122:ILE:N | 1:D:122:ILE:CD1 | 2.79 | 0.45 |
| 1:B:52:ARG:C | 1:B:53:LEU:HD23 | 2.36 | 0.45 |
| 1:C:5:PRO:N | 1:C:114:MET:HE1 | 2.30 | 0.45 |
| 1:B:97:PRO:HG2 | 1:B:108:TRP:HE1 | 1.81 | 0.45 |
| 1:A:78:ASN:C | 1:A:80:ALA:H | 2.19 | 0.45 |
| 1:E:42:GLY:O | 1:E:93:TRP:HA | 2.16 | 0.45 |
| 1:A:18:VAL:HG13 | 1:A:123:GLU:O | 2.16 | 0.45 |
| 1:D:94:THR:OG1 | 1:D:95:ASN:N | 2.50 | 0.45 |
| 1:G:20:ASN:HA | 1:G:125:ASN:HB3 | 1.97 | 0.45 |
| 1:H:55:VAL:CG1 | 1:H:56:ASP:N | 2.79 | 0.45 |
| 1:H:40:ARG:HB3 | 1:H:96:THR:OG1 | 2.17 | 0.45 |
| 1:G:82:GLU:HG2 | 1:G:82:GLU:H | 1.50 | 0.45 |
| 1:G:96:THR:HG22 | 1:G:97:PRO:HD2 | 1.98 | 0.45 |
| 1:F:55:VAL:CG1 | 1:F:56:ASP:H | 2.28 | 0.45 |
| 1:E:19:PHE:CD2 | 1:E:29:TYR:CE1 | 3.05 | 0.45 |
| 1:D:18:VAL:HG13 | 1:D:123:GLU:O | 2.16 | 0.45 |
| 1:H:31:ILE:CG2 | 1:H:32:LYS:N | 2.80 | 0.45 |
| 1:C:120:LEU:HD23 | 1:C:120:LEU:HA | 1.55 | 0.45 |
| 1:C:105:ARG:N | 1:C:108:TRP:CZ3 | 2.78 | 0.45 |
| 1:A:96:THR:CG2 | 1:A:97:PRO:HD2 | 2.47 | 0.45 |
| 1:C:78:ASN:OD1 | 1:C:80:ALA:HB3 | 2.17 | 0.45 |
| 1:C:109:PHE:CD2 | 1:C:115:VAL:HG21 | 2.52 | 0.45 |
| 1:H:6:PRO:HA | 1:H:95:ASN:OD1 | 2.16 | 0.45 |
| 1:E:12:GLN:OE1 | 1:F:22:PRO:HB3 | 2.17 | 0.44 |
| 1:G:4:VAL:HB | 1:G:5:PRO:HD2 | 2.00 | 0.44 |
| 1:E:94:THR:OG1 | 1:E:95:ASN:N | 2.50 | 0.44 |
| 1:B:48:THR:HG22 | 1:B:48:THR:O | 2.17 | 0.44 |
| 1:H:21:ALA:CB | 1:H:22:PRO:HA | 2.28 | 0.44 |
| 1:A:55:VAL:CG1 | 1:A:56:ASP:N | 2.79 | 0.44 |
| 1:H:105:ARG:N | 1:H:108:TRP:CZ3 | 2.79 | 0.44 |
| 1:A:19:PHE:CD2 | 1:A:29:TYR:CE1 | 3.05 | 0.44 |
| 1:G:5:PRO:HA | 1:G:6:PRO:HD3 | 1.81 | 0.44 |
| 1:B:122:ILE:N | 1:B:122:ILE:CD1 | 2.80 | 0.44 |
| 1:D:48:THR:HG22 | 1:D:48:THR:O | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:19:PHE:HA | 1:H:29:TYR:OH | 2.18 | 0.44 |
| 1:B:97:PRO:HG2 | 1:B:108:TRP:NE1 | 2.33 | 0.44 |
| 1:F:55:VAL:CG1 | 1:F:56:ASP:N | 2.79 | 0.44 |
| 1:G:78:ASN:OD1 | 1:G:80:ALA:HB3 | 2.17 | 0.44 |
| 1:E:55:VAL:CG1 | 1:E:56:ASP:H | 2.29 | 0.44 |
| 1:E:68:VAL:CG2 | 1:E:69:LEU:N | 2.80 | 0.44 |
| 1:F:5:PRO:HA | 1:F:6:PRO:HD3 | 1.83 | 0.44 |
| 1:F:109:PHE:CD2 | 1:F:115:VAL:HG21 | 2.52 | 0.44 |
| 1:B:120:LEU:HA | 1:B:120:LEU:HD23 | 1.52 | 0.44 |
| 1:D:55:VAL:CG1 | 1:D:70:MET:HE2 | 2.48 | 0.44 |
| 1:B:68:VAL:HG22 | 1:B:69:LEU:H | 1.81 | 0.44 |
| 1:G:5:PRO:N | 1:G:114:MET:CE | 2.81 | 0.44 |
| 1:F:120:LEU:HA | 1:F:120:LEU:HD23 | 1.50 | 0.44 |
| 1:C:68:VAL:CG2 | 1:C:69:LEU:N | 2.81 | 0.43 |
| 1:C:19:PHE:CD2 | 1:C:29:TYR:CE1 | 3.06 | 0.43 |
| 1:A:97:PRO:CG | 1:A:108:TRP:NE1 | 2.81 | 0.43 |
| 1:E:31:ILE:CG2 | 1:E:32:LYS:N | 2.79 | 0.43 |
| 1:F:114:MET:HE2 | 1:F:114:MET:HB2 | 1.77 | 0.43 |
| 1:B:12:GLN:O | 1:B:31:ILE:HG23 | 2.18 | 0.43 |
| 1:D:4:VAL:HB | 1:D:5:PRO:HD2 | 2.00 | 0.43 |
| 1:A:20:ASN:HA | 1:A:125:ASN:HB3 | 2.00 | 0.43 |
| 1:D:114:MET:HB2 | 1:D:114:MET:HE2 | 1.75 | 0.43 |
| 1:B:76:THR:O | 1:B:77:PHE:HB3 | 2.18 | 0.43 |
| 1:H:52:ARG:C | 1:H:53:LEU:HD23 | 2.38 | 0.43 |
| 1:C:78:ASN:C | 1:C:80:ALA:H | 2.20 | 0.43 |
| 1:F:5:PRO:HA | 1:F:114:MET:CE | 2.47 | 0.43 |
| 1:A:32:LYS:HG3 | 1:A:69:LEU:HD12 | 2.00 | 0.43 |
| 1:B:68:VAL:CG2 | 1:B:69:LEU:N | 2.79 | 0.43 |
| 1:F:105:ARG:N | 1:F:108:TRP:CZ3 | 2.77 | 0.43 |
| 1:H:120:LEU:HD23 | 1:H:120:LEU:HA | 1.55 | 0.43 |
| 1:A:116:ARG:NH1 | 1:A:116:ARG:CG | 2.79 | 0.43 |
| 1:E:55:VAL:CG1 | 1:E:56:ASP:N | 2.81 | 0.43 |
| 1:H:116:ARG:NH1 | 1:H:116:ARG:CG | 2.80 | 0.43 |
| 1:G:76:THR:O | 1:G:77:PHE:HB3 | 2.17 | 0.43 |
| 1:A:122:ILE:CD1 | 1:A:122:ILE:N | 2.80 | 0.43 |
| 1:D:21:ALA:HB1 | 1:D:22:PRO:CA | 2.36 | 0.43 |
| 1:G:114:MET:HB2 | 1:G:114:MET:HE2 | 1.84 | 0.43 |
| 1:C:114:MET:HB2 | 1:C:114:MET:HE2 | 1.82 | 0.43 |
| 1:D:5:PRO:HA | 1:D:6:PRO:HD3 | 1.81 | 0.43 |
| 1:G:68:VAL:CG2 | 1:G:69:LEU:N | 2.81 | 0.43 |
| 1:A:109:PHE:CD2 | 1:A:115:VAL:HG21 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:31:ILE:CG2 | 1:C:32:LYS:N | 2.79 | 0.43 |
| 1:F:68:VAL:CG2 | 1:F:69:LEU:N | 2.79 | 0.43 |
| 1:H:116:ARG:HG2 | 1:H:116:ARG:NH1 | 2.21 | 0.43 |
| 1:A:29:TYR:C | 1:A:30:HIS:ND1 | 2.72 | 0.43 |
| 1:B:31:ILE:CG2 | 1:B:32:LYS:N | 2.80 | 0.43 |
| 1:H:78:ASN:C | 1:H:80:ALA:H | 2.21 | 0.43 |
| 1:H:94:THR:OG1 | 1:H:95:ASN:N | 2.51 | 0.43 |
| 1:C:76:THR:O | 1:C:77:PHE:HB3 | 2.17 | 0.43 |
| 1:E:4:VAL:HB | 1:E:5:PRO:HD2 | 2.01 | 0.43 |
| 1:C:42:GLY:O | 1:C:93:TRP:HA | 2.19 | 0.43 |
| 1:A:57:PRO:HA | 1:A:58:PRO:HD3 | 1.86 | 0.43 |
| 1:H:61:VAL:C | 1:H:62:LEU:HD12 | 2.39 | 0.43 |
| 1:C:18:VAL:HG13 | 1:C:123:GLU:O | 2.18 | 0.43 |
| 1:F:122:ILE:N | 1:F:122:ILE:CD1 | 2.82 | 0.43 |
| 1:A:97:PRO:O | 1:A:99:GLY:N | 2.52 | 0.43 |
| 1:F:4:VAL:HB | 1:F:5:PRO:HD2 | 2.01 | 0.43 |
| 1:H:122:ILE:CD1 | 1:H:122:ILE:N | 2.82 | 0.43 |
| 1:C:4:VAL:HB | 1:C:5:PRO:HD2 | 2.01 | 0.43 |
| 1:E:122:ILE:N | 1:E:122:ILE:CD1 | 2.82 | 0.43 |
| 1:H:32:LYS:HG3 | 1:H:69:LEU:HD12 | 2.01 | 0.43 |
| 1:C:5:PRO:HA | 1:C:6:PRO:HD3 | 1.82 | 0.43 |
| 1:H:68:VAL:HG22 | 1:H:69:LEU:H | 1.84 | 0.42 |
| 1:B:4:VAL:HB | 1:B:5:PRO:HD2 | 2.00 | 0.42 |
| 1:H:76:THR:O | 1:H:77:PHE:HB3 | 2.19 | 0.42 |
| 1:D:55:VAL:CG1 | 1:D:56:ASP:H | 2.30 | 0.42 |
| 1:A:19:PHE:HA | 1:A:29:TYR:OH | 2.18 | 0.42 |
| 1:A:96:THR:CB | 1:A:97:PRO:HD2 | 2.49 | 0.42 |
| 1:D:42:GLY:O | 1:D:93:TRP:HA | 2.20 | 0.42 |
| 1:E:45:ILE:HD12 | 1:E:91:ILE:HG12 | 1.98 | 0.42 |
| 1:B:19:PHE:CD2 | 1:B:29:TYR:CE1 | 3.07 | 0.42 |
| 1:A:17:ILE:HD12 | 1:A:19:PHE:HE1 | 1.83 | 0.42 |
| 1:E:32:LYS:HG3 | 1:E:69:LEU:HD12 | 2.01 | 0.42 |
| 1:D:12:GLN:O | 1:D:31:ILE:HG23 | 2.18 | 0.42 |
| 1:H:5:PRO:N | 1:H:114:MET:HE1 | 2.34 | 0.42 |
| 1:H:4:VAL:HB | 1:H:5:PRO:HD2 | 2.00 | 0.42 |
| 1:G:68:VAL:HG22 | 1:G:69:LEU:H | 1.84 | 0.42 |
| 1:G:12:GLN:O | 1:G:31:ILE:HG23 | 2.19 | 0.42 |
| 1:E:116:ARG:NH1 | 1:E:116:ARG:CG | 2.79 | 0.42 |
| 1:C:55:VAL:CG1 | 1:C:56:ASP:H | 2.28 | 0.42 |
| 1:D:105:ARG:N | 1:D:108:TRP:CZ3 | 2.79 | 0.42 |
| 1:C:68:VAL:HG22 | 1:C:69:LEU:H | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:32:LYS:HG3 | 1:F:69:LEU:HD12 | 2.01 | 0.42 |
| 1:F:116:ARG:NH1 | 1:F:116:ARG:CG | 2.80 | 0.42 |
| 1:B:116:ARG:NH1 | 1:B:116:ARG:CG | 2.80 | 0.42 |
| 1:G:5:PRO:CA | 1:G:114:MET:HE3 | 2.48 | 0.42 |
| 1:A:4:VAL:HB | 1:A:5:PRO:HD2 | 2.00 | 0.42 |
| 1:D:116:ARG:CG | 1:D:116:ARG:NH1 | 2.80 | 0.42 |
| 1:H:68:VAL:CG2 | 1:H:69:LEU:N | 2.82 | 0.42 |
| 1:B:96:THR:CG2 | 1:B:97:PRO:HD2 | 2.49 | 0.42 |
| 1:G:109:PHE:CD2 | 1:G:115:VAL:HG21 | 2.54 | 0.42 |
| 1:F:31:ILE:CG2 | 1:F:32:LYS:N | 2.82 | 0.42 |
| 1:B:43:TRP:CD1 | 1:B:62:LEU:HD13 | 2.55 | 0.42 |
| 1:E:29:TYR:C | 1:E:30:HIS:ND1 | 2.73 | 0.42 |
| 1:C:94:THR:OG1 | 1:C:95:ASN:N | 2.52 | 0.42 |
| 1:F:45:ILE:CG1 | 1:F:70:MET:HE1 | 2.41 | 0.42 |
| 1:F:12:GLN:O | 1:F:31:ILE:HG23 | 2.20 | 0.41 |
| 1:G:6:PRO:HA | 1:G:95:ASN:OD1 | 2.20 | 0.41 |
| 1:C:40:ARG:HB3 | 1:C:96:THR:OG1 | 2.20 | 0.41 |
| 1:F:68:VAL:HG22 | 1:F:69:LEU:H | 1.82 | 0.41 |
| 1:G:45:ILE:HD12 | 1:G:91:ILE:HG12 | 1.99 | 0.41 |
| 1:A:40:ARG:NH1 | 1:A:102:LYS:HG3 | 2.34 | 0.41 |
| 1:H:91:ILE:O | 1:H:117:ARG:HA | 2.20 | 0.41 |
| 1:H:5:PRO:CA | 1:H:114:MET:HE3 | 2.49 | 0.41 |
| 1:A:94:THR:OG1 | 1:A:95:ASN:N | 2.52 | 0.41 |
| 1:D:29:TYR:C | 1:D:30:HIS:ND1 | 2.74 | 0.41 |
| 1:E:19:PHE:HA | 1:E:29:TYR:OH | 2.20 | 0.41 |
| 1:D:77:PHE:CD2 | 1:D:78:ASN:N | 2.89 | 0.41 |
| 1:H:29:TYR:C | 1:H:30:HIS:ND1 | 2.74 | 0.41 |
| 1:A:78:ASN:C | 1:A:80:ALA:N | 2.72 | 0.41 |
| 1:D:32:LYS:HG3 | 1:D:69:LEU:HD12 | 2.02 | 0.41 |
| 1:G:104:PHE:CE1 | 1:G:109:PHE:HE1 | 2.39 | 0.41 |
| 1:D:97:PRO:O | 1:D:99:GLY:N | 2.54 | 0.41 |
| 1:B:5:PRO:HA | 1:B:114:MET:HE3 | 2.01 | 0.41 |
| 1:A:21:ALA:CB | 1:A:22:PRO:HA | 2.30 | 0.41 |
| 1:H:55:VAL:CG1 | 1:H:70:MET:CE | 2.97 | 0.41 |
| 1:F:82:GLU:O | 1:F:84:LEU:HG | 2.20 | 0.41 |
| 1:H:18:VAL:HG13 | 1:H:123:GLU:O | 2.21 | 0.41 |
| 1:F:6:PRO:HA | 1:F:95:ASN:OD1 | 2.20 | 0.41 |
| 1:A:31:ILE:CG2 | 1:A:32:LYS:N | 2.83 | 0.41 |
| 1:E:56:ASP:HA | 1:E:57:PRO:HA | 1.87 | 0.41 |
| 1:G:57:PRO:HA | 1:G:58:PRO:HD3 | 1.85 | 0.41 |
| 1:F:29:TYR:C | 1:F:30:HIS:ND1 | 2.74 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:97:PRO:HG2 | 1:E:108:TRP:HE1 | 1.85 | 0.41 |
| 1:E:40:ARG:HB3 | 1:E:96:THR:OG1 | 2.20 | 0.41 |
| 1:B:32:LYS:HG3 | 1:B:69:LEU:HD12 | 2.03 | 0.41 |
| 1:G:19:PHE:HA | 1:G:29:TYR:OH | 2.21 | 0.41 |
| 1:C:97:PRO:O | 1:C:99:GLY:N | 2.54 | 0.41 |
| 1:B:109:PHE:CD2 | 1:B:115:VAL:HG21 | 2.56 | 0.41 |
| 1:A:55:VAL:CG1 | 1:A:70:MET:HE2 | 2.49 | 0.40 |
| 1:F:43:TRP:HA | 1:F:92:GLU:O | 2.21 | 0.40 |
| 1:C:5:PRO:N | 1:C:114:MET:CE | 2.85 | 0.40 |
| 1:H:46:LYS:O | 1:H:90:CYS:N | 2.46 | 0.40 |
| 1:E:101:ALA:O | 1:E:103:GLN:N | 2.54 | 0.40 |
| 1:C:104:PHE:CE1 | 1:C:109:PHE:HE1 | 2.40 | 0.40 |
| 1:B:5:PRO:HA | 1:B:6:PRO:HD3 | 1.82 | 0.40 |
| 1:C:12:GLN:O | 1:C:31:ILE:HG23 | 2.21 | 0.40 |
| 1:B:19:PHE:HA | 1:B:29:TYR:OH | 2.20 | 0.40 |
| 1:A:5:PRO:HA | 1:A:6:PRO:HD3 | 1.82 | 0.40 |
| 1:C:32:LYS:HG3 | 1:C:69:LEU:HD12 | 2.02 | 0.40 |
| 1:E:61:VAL:C | 1:E:62:LEU:HD12 | 2.42 | 0.40 |
| 1:C:119:ASN:HB2 | 1:D:112:ASP:OD1 | 2.21 | 0.40 |
| 1:A:12:GLN:O | 1:A:31:ILE:HG23 | 2.22 | 0.40 |
| 1:B:96:THR:CB | 1:B:97:PRO:HD2 | 2.51 | 0.40 |
| 1:G:122:ILE:CD1 | 1:G:122:ILE:N | 2.82 | 0.40 |
| 1:H:45:ILE:HD12 | 1:H:91:ILE:HG12 | 2.00 | 0.40 |
| 1:E:45:ILE:HA | 1:E:45:ILE:HD13 | 1.91 | 0.40 |
| 1:E:45:ILE:CG2 | 1:E:46:LYS:N | 2.83 | 0.40 |
| 1:B:17:ILE:HD12 | 1:B:19:PHE:HE1 | 1.86 | 0.40 |
| 1:B:29:TYR:C | 1:B:30:HIS:ND1 | 2.74 | 0.40 |
| 1:G:53:LEU:N | 1:G:53:LEU:CD2 | 2.75 | 0.40 |
| 1:E:5:PRO:HA | 1:E:6:PRO:HD3 | 1.79 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|-----------|----------|-------------|----|
| 1 | A | 122/126 (97%) | 103 (84%) | 14 (12%) | 5 (4%) | 3 | 24 |
| 1 | B | 122/126 (97%) | 103 (84%) | 15 (12%) | 4 (3%) | 5 | 30 |
| 1 | C | 122/126 (97%) | 102 (84%) | 16 (13%) | 4 (3%) | 5 | 30 |
| 1 | D | 122/126 (97%) | 103 (84%) | 15 (12%) | 4 (3%) | 5 | 30 |
| 1 | E | 122/126 (97%) | 104 (85%) | 15 (12%) | 3 (2%) | 7 | 37 |
| 1 | F | 122/126 (97%) | 102 (84%) | 16 (13%) | 4 (3%) | 5 | 30 |
| 1 | G | 122/126 (97%) | 103 (84%) | 15 (12%) | 4 (3%) | 5 | 30 |
| 1 | H | 122/126 (97%) | 103 (84%) | 17 (14%) | 2 (2%) | 12 | 48 |
| All | All | 976/1008 (97%) | 823 (84%) | 123 (13%) | 30 (3%) | 5 | 32 |

All (30) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 79 | ALA |
| 1 | A | 98 | ASP |
| 1 | B | 98 | ASP |
| 1 | C | 79 | ALA |
| 1 | C | 98 | ASP |
| 1 | C | 111 | GLY |
| 1 | D | 98 | ASP |
| 1 | E | 98 | ASP |
| 1 | F | 98 | ASP |
| 1 | A | 111 | GLY |
| 1 | B | 79 | ALA |
| 1 | D | 102 | LYS |
| 1 | D | 111 | GLY |
| 1 | F | 79 | ALA |
| 1 | G | 79 | ALA |
| 1 | G | 98 | ASP |
| 1 | G | 111 | GLY |
| 1 | H | 79 | ALA |
| 1 | A | 102 | LYS |
| 1 | F | 15 | SER |
| 1 | H | 15 | SER |
| 1 | A | 15 | SER |
| 1 | B | 15 | SER |
| 1 | B | 40 | ARG |
| 1 | C | 15 | SER |
| 1 | D | 15 | SER |
| 1 | E | 15 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 102 | LYS |
| 1 | G | 15 | SER |
| 1 | F | 111 | GLY |

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 | 106/107 (99%) | 81 (76%) | 25 (24%) | 1 | 3 |
| 1 | B | 106/107 (99%) | 82 (77%) | 24 (23%) | 1 | 4 |
| 1 | C | 106/107 (99%) | 80 (76%) | 26 (24%) | 1 | 3 |
| 1 | D | 106/107 (99%) | 80 (76%) | 26 (24%) | 1 | 3 |
| 1 | E | 106/107 (99%) | 81 (76%) | 25 (24%) | 1 | 3 |
| 1 | F | 106/107 (99%) | 81 (76%) | 25 (24%) | 1 | 3 |
| 1 | G | 106/107 (99%) | 81 (76%) | 25 (24%) | 1 | 3 |
| 1 | H | 106/107 (99%) | 82 (77%) | 24 (23%) | 1 | 4 |
| All | All | 848/856 (99%) | 648 (76%) | 200 (24%) | 1 | 3 |

All (200) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 8 | ASP |
| 1 | A | 9 | ILE |
| 1 | A | 15 | SER |
| 1 | A | 17 | ILE |
| 1 | A | 30 | HIS |
| 1 | A | 32 | LYS |
| 1 | A | 34 | THR |
| 1 | A | 40 | ARG |
| 1 | A | 50 | MET |
| 1 | A | 53 | LEU |
| 1 | A | 67 | LYS |
| 1 | A | 70 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 73 | SER |
| 1 | A | 76 | THR |
| 1 | A | 84 | LEU |
| 1 | A | 85 | ASN |
| 1 | A | 88 | ARG |
| 1 | A | 89 | ILE |
| 1 | A | 96 | THR |
| 1 | A | 106 | ARG |
| 1 | A | 112 | ASP |
| 1 | A | 114 | MET |
| 1 | A | 115 | VAL |
| 1 | A | 116 | ARG |
| 1 | A | 122 | ILE |
| 1 | B | 8 | ASP |
| 1 | B | 9 | ILE |
| 1 | B | 15 | SER |
| 1 | B | 17 | ILE |
| 1 | B | 24 | ASP |
| 1 | B | 25 | ASP |
| 1 | B | 32 | LYS |
| 1 | B | 34 | THR |
| 1 | B | 40 | ARG |
| 1 | B | 50 | MET |
| 1 | B | 67 | LYS |
| 1 | B | 70 | MET |
| 1 | B | 73 | SER |
| 1 | B | 76 | THR |
| 1 | B | 81 | THR |
| 1 | B | 84 | LEU |
| 1 | B | 85 | ASN |
| 1 | B | 88 | ARG |
| 1 | B | 89 | ILE |
| 1 | B | 96 | THR |
| 1 | B | 106 | ARG |
| 1 | B | 114 | MET |
| 1 | B | 116 | ARG |
| 1 | B | 122 | ILE |
| 1 | C | 8 | ASP |
| 1 | C | 9 | ILE |
| 1 | C | 15 | SER |
| 1 | C | 17 | ILE |
| 1 | C | 24 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 25 | ASP |
| 1 | C | 30 | HIS |
| 1 | C | 32 | LYS |
| 1 | C | 34 | THR |
| 1 | C | 40 | ARG |
| 1 | C | 50 | MET |
| 1 | C | 53 | LEU |
| 1 | C | 67 | LYS |
| 1 | C | 70 | MET |
| 1 | C | 73 | SER |
| 1 | C | 76 | THR |
| 1 | C | 82 | GLU |
| 1 | C | 84 | LEU |
| 1 | C | 85 | ASN |
| 1 | C | 88 | ARG |
| 1 | C | 89 | ILE |
| 1 | C | 96 | THR |
| 1 | C | 106 | ARG |
| 1 | C | 114 | MET |
| 1 | C | 116 | ARG |
| 1 | C | 122 | ILE |
| 1 | D | 6 | PRO |
| 1 | D | 8 | ASP |
| 1 | D | 9 | ILE |
| 1 | D | 15 | SER |
| 1 | D | 17 | ILE |
| 1 | D | 24 | ASP |
| 1 | D | 25 | ASP |
| 1 | D | 32 | LYS |
| 1 | D | 34 | THR |
| 1 | D | 40 | ARG |
| 1 | D | 50 | MET |
| 1 | D | 67 | LYS |
| 1 | D | 70 | MET |
| 1 | D | 73 | SER |
| 1 | D | 76 | THR |
| 1 | D | 81 | THR |
| 1 | D | 84 | LEU |
| 1 | D | 85 | ASN |
| 1 | D | 88 | ARG |
| 1 | D | 89 | ILE |
| 1 | D | 96 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 106 | ARG |
| 1 | D | 112 | ASP |
| 1 | D | 114 | MET |
| 1 | D | 116 | ARG |
| 1 | D | 122 | ILE |
| 1 | E | 8 | ASP |
| 1 | E | 9 | ILE |
| 1 | E | 15 | SER |
| 1 | E | 17 | ILE |
| 1 | E | 24 | ASP |
| 1 | E | 25 | ASP |
| 1 | E | 30 | HIS |
| 1 | E | 32 | LYS |
| 1 | E | 34 | THR |
| 1 | E | 40 | ARG |
| 1 | E | 50 | MET |
| 1 | E | 53 | LEU |
| 1 | E | 67 | LYS |
| 1 | E | 70 | MET |
| 1 | E | 73 | SER |
| 1 | E | 76 | THR |
| 1 | E | 84 | LEU |
| 1 | E | 85 | ASN |
| 1 | E | 88 | ARG |
| 1 | E | 89 | ILE |
| 1 | E | 96 | THR |
| 1 | E | 106 | ARG |
| 1 | E | 114 | MET |
| 1 | E | 116 | ARG |
| 1 | E | 122 | ILE |
| 1 | F | 8 | ASP |
| 1 | F | 9 | ILE |
| 1 | F | 15 | SER |
| 1 | F | 17 | ILE |
| 1 | F | 24 | ASP |
| 1 | F | 25 | ASP |
| 1 | F | 32 | LYS |
| 1 | F | 34 | THR |
| 1 | F | 40 | ARG |
| 1 | F | 50 | MET |
| 1 | F | 67 | LYS |
| 1 | F | 70 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 73 | SER |
| 1 | F | 76 | THR |
| 1 | F | 84 | LEU |
| 1 | F | 85 | ASN |
| 1 | F | 88 | ARG |
| 1 | F | 89 | ILE |
| 1 | F | 96 | THR |
| 1 | F | 106 | ARG |
| 1 | F | 112 | ASP |
| 1 | F | 114 | MET |
| 1 | F | 115 | VAL |
| 1 | F | 116 | ARG |
| 1 | F | 122 | ILE |
| 1 | G | 8 | ASP |
| 1 | G | 9 | ILE |
| 1 | G | 15 | SER |
| 1 | G | 17 | ILE |
| 1 | G | 24 | ASP |
| 1 | G | 25 | ASP |
| 1 | G | 32 | LYS |
| 1 | G | 34 | THR |
| 1 | G | 40 | ARG |
| 1 | G | 50 | MET |
| 1 | G | 67 | LYS |
| 1 | G | 70 | MET |
| 1 | G | 73 | SER |
| 1 | G | 76 | THR |
| 1 | G | 82 | GLU |
| 1 | G | 84 | LEU |
| 1 | G | 85 | ASN |
| 1 | G | 88 | ARG |
| 1 | G | 89 | ILE |
| 1 | G | 96 | THR |
| 1 | G | 106 | ARG |
| 1 | G | 112 | ASP |
| 1 | G | 114 | MET |
| 1 | G | 116 | ARG |
| 1 | G | 122 | ILE |
| 1 | H | 8 | ASP |
| 1 | H | 15 | SER |
| 1 | H | 17 | ILE |
| 1 | H | 24 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 25 | ASP |
| 1 | H | 32 | LYS |
| 1 | H | 34 | THR |
| 1 | H | 39 | ARG |
| 1 | H | 40 | ARG |
| 1 | H | 50 | MET |
| 1 | H | 67 | LYS |
| 1 | H | 70 | MET |
| 1 | H | 73 | SER |
| 1 | H | 76 | THR |
| 1 | H | 84 | LEU |
| 1 | H | 85 | ASN |
| 1 | H | 88 | ARG |
| 1 | H | 89 | ILE |
| 1 | H | 96 | THR |
| 1 | H | 106 | ARG |
| 1 | H | 114 | MET |
| 1 | H | 116 | ARG |
| 1 | H | 117 | ARG |
| 1 | H | 122 | ILE |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 27 | HIS |
| 1 | A | 85 | ASN |
| 1 | B | 27 | HIS |
| 1 | B | 85 | ASN |
| 1 | C | 27 | HIS |
| 1 | C | 85 | ASN |
| 1 | D | 27 | HIS |
| 1 | D | 85 | ASN |
| 1 | D | 119 | ASN |
| 1 | E | 27 | HIS |
| 1 | E | 85 | ASN |
| 1 | F | 27 | HIS |
| 1 | F | 85 | ASN |
| 1 | G | 27 | HIS |
| 1 | G | 85 | ASN |
| 1 | H | 27 | HIS |
| 1 | H | 85 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.