



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:17 PM UTC

PDB ID : 1IOI / pdb\_00001ioi  
Title : x-ray crystalline structures of pyrrolidone carboxyl peptidase from a hyper-thermophile, *pyrococcus furiosus*, and its cys-free mutant  
Authors : Tanaka, H.; Chinami, M.; Ota, M.; Tsukihara, T.; Yutani, K.  
Deposited on : 2001-03-09  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

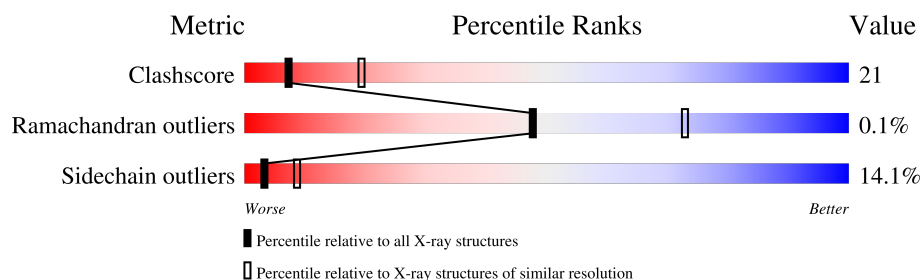
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

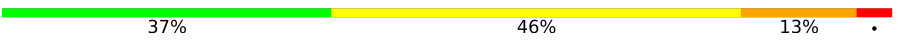
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 3843 (2.70-2.70)                                      |
| Ramachandran outliers | 187476                      | 3778 (2.70-2.70)                                      |
| Sidechain outliers    | 187428                      | 3778 (2.70-2.70)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain                                                                                    |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------|
| 1   | A     | 208    |  37% 46% 13% .  |
| 1   | B     | 208    |  41% 41% 14% .  |
| 1   | C     | 208    |  40% 42% 13% .  |
| 1   | D     | 208    |  37% 43% 15% 5% |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6544 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 PYRROLIDONE CARBOXYL PEPTIDASE.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1605  | 1040 | 263 | 296 | 6 |         |         |       |
| 1   | B     | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1605  | 1040 | 263 | 296 | 6 |         |         |       |
| 1   | C     | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1605  | 1040 | 263 | 296 | 6 |         |         |       |
| 1   | D     | 208      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1605  | 1040 | 263 | 296 | 6 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 142     | SER      | CYS    | engineered mutation | UNP O73944 |
| A     | 188     | SER      | CYS    | engineered mutation | UNP O73944 |
| B     | 142     | SER      | CYS    | engineered mutation | UNP O73944 |
| B     | 188     | SER      | CYS    | engineered mutation | UNP O73944 |
| C     | 142     | SER      | CYS    | engineered mutation | UNP O73944 |
| C     | 188     | SER      | CYS    | engineered mutation | UNP O73944 |
| D     | 142     | SER      | CYS    | engineered mutation | UNP O73944 |
| D     | 188     | SER      | CYS    | engineered mutation | UNP O73944 |

- Molecule 2 is water.

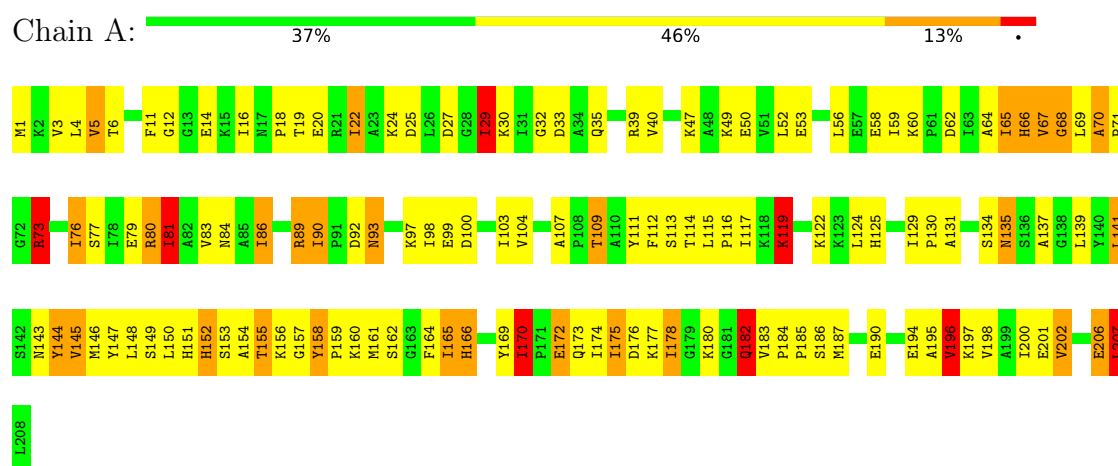
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 30       | Total | O  | 0       | 0       |
|     |       |          | 30    | 30 |         |         |
| 2   | B     | 34       | Total | O  | 0       | 0       |
|     |       |          | 34    | 34 |         |         |
| 2   | C     | 28       | Total | O  | 0       | 0       |
|     |       |          | 28    | 28 |         |         |
| 2   | D     | 32       | Total | O  | 0       | 0       |
|     |       |          | 32    | 32 |         |         |

### 3 Residue-property plots

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

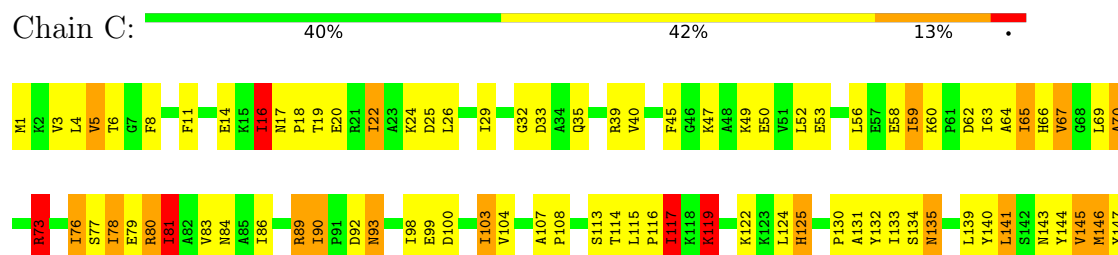
#### • Molecule 1: PYRROLIDONE CARBOXYL PEPTIDASE



#### • Molecule 1: PYRROLIDONE CARBOXYL PEPTIDASE

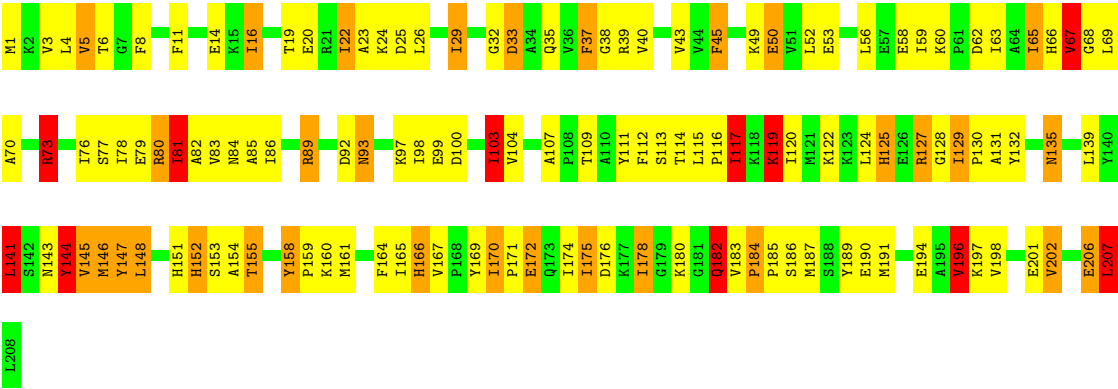


#### • Molecule 1: PYRROLIDONE CARBOXYL PEPTIDASE





● Molecule 1: PYRROLIDONE CARBOXYL PEPTIDASE



## 4 Data and refinement statistics

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

| Property                                                 | Value                                                     | Source    |
|----------------------------------------------------------|-----------------------------------------------------------|-----------|
| Space group                                              | P 1 21 1                                                  | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 49.00 Å   105.80 Å   105.80 Å<br>90.00°   96.20°   90.00° | Depositor |
| Resolution (Å)                                           | 10.00 – 2.70                                              | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) (10.00-2.70)                              | Depositor |
| $R_{merge}$                                              | 0.13                                                      | Depositor |
| $R_{sym}$                                                | (Not available)                                           | Depositor |
| Refinement program                                       | X-PLOR                                                    | Depositor |
| R, $R_{free}$                                            | 0.210 , 0.243                                             | Depositor |
| Estimated twinning fraction                              | No twinning to report.                                    | Xtriage   |
| Total number of atoms                                    | 6544                                                      | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 26.0                                                      | 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     | 1.80         | 30/1639 (1.8%)  | 2.23        | 78/2216 (3.5%)  |
| 1   | B     | 1.76         | 31/1639 (1.9%)  | 2.25        | 85/2216 (3.8%)  |
| 1   | C     | 1.78         | 31/1639 (1.9%)  | 2.24        | 87/2216 (3.9%)  |
| 1   | D     | 1.78         | 29/1639 (1.8%)  | 2.25        | 82/2216 (3.7%)  |
| All | All   | 1.78         | 121/6556 (1.8%) | 2.24        | 332/8864 (3.7%) |

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                   | 1                   |
| 1   | B     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

All (121) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | C     | 60  | LYS  | CA-CB   | 16.55  | 1.64        | 1.52     |
| 1   | D     | 196 | VAL  | CA-CB   | 11.98  | 1.71        | 1.54     |
| 1   | D     | 202 | VAL  | CA-CB   | 11.48  | 1.69        | 1.54     |
| 1   | A     | 60  | LYS  | CA-CB   | 11.34  | 1.62        | 1.52     |
| 1   | B     | 202 | VAL  | CA-CB   | 10.78  | 1.69        | 1.54     |
| 1   | D     | 60  | LYS  | CA-CB   | 10.55  | 1.61        | 1.52     |
| 1   | C     | 202 | VAL  | CA-CB   | 10.47  | 1.68        | 1.54     |
| 1   | A     | 196 | VAL  | CA-CB   | 10.45  | 1.69        | 1.54     |
| 1   | C     | 196 | VAL  | CA-CB   | 10.41  | 1.69        | 1.54     |
| 1   | A     | 202 | VAL  | CA-CB   | 10.26  | 1.68        | 1.54     |
| 1   | B     | 66  | HIS  | CD2-NE2 | -10.16 | 1.26        | 1.37     |
| 1   | D     | 175 | ILE  | CA-CB   | 10.02  | 1.69        | 1.54     |
| 1   | C     | 66  | HIS  | CD2-NE2 | -9.76  | 1.27        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 60  | LYS  | CA-CB   | 9.51  | 1.60        | 1.52     |
| 1   | B     | 152 | HIS  | CD2-NE2 | -9.31 | 1.27        | 1.37     |
| 1   | C     | 152 | HIS  | CD2-NE2 | -9.30 | 1.27        | 1.37     |
| 1   | B     | 166 | HIS  | CD2-NE2 | -9.23 | 1.27        | 1.37     |
| 1   | A     | 175 | ILE  | CA-CB   | 9.06  | 1.67        | 1.54     |
| 1   | B     | 175 | ILE  | CA-CB   | 9.06  | 1.67        | 1.54     |
| 1   | B     | 196 | VAL  | CA-CB   | 9.00  | 1.67        | 1.54     |
| 1   | A     | 66  | HIS  | CD2-NE2 | -8.87 | 1.28        | 1.37     |
| 1   | C     | 175 | ILE  | CA-CB   | 8.69  | 1.67        | 1.54     |
| 1   | D     | 166 | HIS  | CD2-NE2 | -8.52 | 1.28        | 1.37     |
| 1   | C     | 166 | HIS  | CD2-NE2 | -8.48 | 1.28        | 1.37     |
| 1   | C     | 151 | HIS  | CD2-NE2 | -8.44 | 1.28        | 1.37     |
| 1   | A     | 166 | HIS  | CD2-NE2 | -8.31 | 1.28        | 1.37     |
| 1   | B     | 125 | HIS  | CD2-NE2 | -8.14 | 1.28        | 1.37     |
| 1   | A     | 40  | VAL  | CA-CB   | 7.99  | 1.63        | 1.54     |
| 1   | D     | 125 | HIS  | CD2-NE2 | -7.70 | 1.29        | 1.37     |
| 1   | B     | 81  | ILE  | CA-CB   | 7.35  | 1.64        | 1.54     |
| 1   | A     | 145 | VAL  | CA-CB   | 7.33  | 1.64        | 1.54     |
| 1   | C     | 16  | ILE  | CA-CB   | 7.32  | 1.65        | 1.55     |
| 1   | B     | 167 | VAL  | CA-CB   | 7.30  | 1.63        | 1.54     |
| 1   | A     | 125 | HIS  | CD2-NE2 | -7.29 | 1.29        | 1.37     |
| 1   | B     | 22  | ILE  | CA-CB   | 7.27  | 1.63        | 1.54     |
| 1   | C     | 59  | ILE  | CA-CB   | 7.23  | 1.65        | 1.54     |
| 1   | B     | 145 | VAL  | CA-CB   | 7.12  | 1.64        | 1.54     |
| 1   | A     | 109 | THR  | CA-CB   | 7.12  | 1.64        | 1.53     |
| 1   | D     | 40  | VAL  | CA-CB   | 7.11  | 1.62        | 1.54     |
| 1   | A     | 81  | ILE  | CA-CB   | 7.03  | 1.63        | 1.54     |
| 1   | C     | 158 | TYR  | CA-C    | 6.98  | 1.59        | 1.52     |
| 1   | D     | 145 | VAL  | CA-CB   | 6.97  | 1.63        | 1.54     |
| 1   | D     | 152 | HIS  | CD2-NE2 | -6.90 | 1.30        | 1.37     |
| 1   | D     | 167 | VAL  | CA-CB   | 6.86  | 1.63        | 1.54     |
| 1   | C     | 125 | HIS  | CD2-NE2 | -6.80 | 1.30        | 1.37     |
| 1   | A     | 183 | VAL  | CA-CB   | 6.71  | 1.62        | 1.54     |
| 1   | B     | 117 | ILE  | CA-CB   | 6.66  | 1.62        | 1.54     |
| 1   | C     | 145 | VAL  | CA-CB   | 6.66  | 1.63        | 1.54     |
| 1   | D     | 19  | THR  | CA-CB   | 6.56  | 1.64        | 1.53     |
| 1   | C     | 19  | THR  | CA-CB   | 6.54  | 1.64        | 1.53     |
| 1   | B     | 59  | ILE  | CA-CB   | 6.51  | 1.63        | 1.54     |
| 1   | B     | 185 | PRO  | C-O     | 6.49  | 1.31        | 1.23     |
| 1   | B     | 151 | HIS  | CD2-NE2 | -6.44 | 1.30        | 1.37     |
| 1   | A     | 19  | THR  | CA-CB   | 6.42  | 1.63        | 1.53     |
| 1   | D     | 66  | HIS  | CD2-NE2 | -6.38 | 1.30        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 158 | TYR  | CA-C    | 6.38  | 1.58        | 1.52     |
| 1   | B     | 66  | HIS  | CG-ND1  | -6.35 | 1.31        | 1.38     |
| 1   | C     | 81  | ILE  | CA-CB   | 6.34  | 1.62        | 1.54     |
| 1   | B     | 76  | ILE  | CA-CB   | 6.32  | 1.61        | 1.53     |
| 1   | D     | 22  | ILE  | CA-CB   | 6.30  | 1.62        | 1.54     |
| 1   | A     | 114 | THR  | CA-CB   | 6.22  | 1.64        | 1.53     |
| 1   | B     | 171 | PRO  | CA-CB   | -6.21 | 1.44        | 1.53     |
| 1   | D     | 81  | ILE  | CA-CB   | 6.21  | 1.62        | 1.54     |
| 1   | B     | 19  | THR  | CA-CB   | 6.20  | 1.63        | 1.53     |
| 1   | D     | 151 | HIS  | CD2-NE2 | -6.19 | 1.31        | 1.37     |
| 1   | C     | 183 | VAL  | CA-CB   | 6.16  | 1.62        | 1.54     |
| 1   | A     | 117 | ILE  | CA-CB   | 6.02  | 1.63        | 1.54     |
| 1   | C     | 117 | ILE  | CA-CB   | 6.02  | 1.63        | 1.54     |
| 1   | C     | 40  | VAL  | CA-CB   | 6.01  | 1.61        | 1.54     |
| 1   | C     | 151 | HIS  | CG-ND1  | -5.98 | 1.31        | 1.38     |
| 1   | A     | 67  | VAL  | CA-CB   | 5.93  | 1.63        | 1.54     |
| 1   | C     | 133 | ILE  | CA-CB   | 5.90  | 1.60        | 1.53     |
| 1   | D     | 67  | VAL  | CA-CB   | 5.88  | 1.63        | 1.54     |
| 1   | A     | 20  | GLU  | CA-CB   | -5.85 | 1.44        | 1.53     |
| 1   | B     | 60  | LYS  | C-O     | 5.85  | 1.26        | 1.23     |
| 1   | B     | 114 | THR  | CA-CB   | 5.82  | 1.64        | 1.53     |
| 1   | C     | 67  | VAL  | CA-CB   | 5.77  | 1.63        | 1.54     |
| 1   | A     | 16  | ILE  | CA-CB   | 5.72  | 1.63        | 1.55     |
| 1   | C     | 125 | HIS  | CG-CD2  | 5.69  | 1.42        | 1.35     |
| 1   | A     | 152 | HIS  | CD2-NE2 | -5.68 | 1.31        | 1.37     |
| 1   | A     | 162 | SER  | CA-C    | 5.66  | 1.59        | 1.52     |
| 1   | D     | 114 | THR  | CA-CB   | 5.61  | 1.63        | 1.53     |
| 1   | D     | 80  | ARG  | CA-C    | 5.60  | 1.60        | 1.52     |
| 1   | D     | 183 | VAL  | CA-CB   | 5.58  | 1.61        | 1.54     |
| 1   | D     | 132 | TYR  | CA-CB   | 5.57  | 1.63        | 1.53     |
| 1   | B     | 20  | GLU  | CA-CB   | -5.56 | 1.44        | 1.53     |
| 1   | C     | 66  | HIS  | CG-ND1  | -5.55 | 1.32        | 1.38     |
| 1   | A     | 76  | ILE  | CA-CB   | 5.53  | 1.60        | 1.53     |
| 1   | A     | 152 | HIS  | CG-CD2  | 5.52  | 1.42        | 1.35     |
| 1   | B     | 40  | VAL  | CA-CB   | 5.51  | 1.60        | 1.54     |
| 1   | B     | 16  | ILE  | CA-CB   | 5.50  | 1.63        | 1.55     |
| 1   | B     | 158 | TYR  | CA-C    | 5.48  | 1.58        | 1.52     |
| 1   | D     | 16  | ILE  | CA-CB   | 5.44  | 1.63        | 1.55     |
| 1   | C     | 60  | LYS  | C-O     | 5.44  | 1.26        | 1.23     |
| 1   | B     | 132 | TYR  | CA-CB   | 5.43  | 1.63        | 1.53     |
| 1   | D     | 117 | ILE  | CA-CB   | 5.42  | 1.62        | 1.54     |
| 1   | A     | 29  | ILE  | CA-CB   | 5.41  | 1.61        | 1.54     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 78  | ILE  | CA-CB | 5.31  | 1.59        | 1.53     |
| 1   | D     | 185 | PRO  | C-O   | 5.31  | 1.29        | 1.23     |
| 1   | D     | 170 | ILE  | CA-CB | 5.27  | 1.60        | 1.54     |
| 1   | D     | 147 | TYR  | CA-CB | 5.26  | 1.62        | 1.53     |
| 1   | D     | 169 | TYR  | CA-CB | -5.26 | 1.44        | 1.53     |
| 1   | C     | 134 | SER  | CA-C  | 5.25  | 1.59        | 1.52     |
| 1   | A     | 83  | VAL  | CA-CB | 5.20  | 1.62        | 1.55     |
| 1   | A     | 150 | LEU  | CA-C  | 5.20  | 1.59        | 1.52     |
| 1   | D     | 158 | TYR  | CA-C  | 5.19  | 1.57        | 1.52     |
| 1   | D     | 184 | PRO  | CA-C  | 5.18  | 1.55        | 1.52     |
| 1   | C     | 150 | LEU  | CA-C  | 5.15  | 1.59        | 1.52     |
| 1   | B     | 78  | ILE  | CA-CB | 5.15  | 1.59        | 1.53     |
| 1   | B     | 162 | SER  | CA-C  | 5.15  | 1.58        | 1.52     |
| 1   | D     | 103 | ILE  | CA-CB | 5.15  | 1.60        | 1.54     |
| 1   | A     | 185 | PRO  | C-O   | 5.14  | 1.29        | 1.23     |
| 1   | A     | 134 | SER  | CA-C  | 5.14  | 1.59        | 1.52     |
| 1   | B     | 67  | VAL  | CA-CB | 5.13  | 1.62        | 1.54     |
| 1   | A     | 27  | ASP  | N-CA  | -5.12 | 1.39        | 1.46     |
| 1   | B     | 133 | ILE  | CA-CB | 5.09  | 1.59        | 1.53     |
| 1   | A     | 157 | GLY  | CA-C  | 5.09  | 1.58        | 1.51     |
| 1   | C     | 167 | VAL  | CA-CB | 5.08  | 1.60        | 1.54     |
| 1   | C     | 76  | ILE  | CA-CB | 5.05  | 1.61        | 1.53     |
| 1   | C     | 169 | TYR  | C-N   | -5.03 | 1.27        | 1.33     |
| 1   | C     | 132 | TYR  | CA-CB | 5.02  | 1.62        | 1.53     |

All (332) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | C     | 103 | ILE  | N-CA-C     | -11.09 | 100.65      | 110.74   |
| 1   | B     | 201 | GLU  | CA-C-O     | -10.73 | 109.17      | 120.55   |
| 1   | D     | 103 | ILE  | N-CA-C     | -10.46 | 101.22      | 110.74   |
| 1   | B     | 103 | ILE  | N-CA-C     | -9.54  | 102.06      | 110.74   |
| 1   | C     | 201 | GLU  | CA-C-O     | -9.52  | 110.45      | 120.55   |
| 1   | A     | 103 | ILE  | N-CA-C     | -8.93  | 102.61      | 110.74   |
| 1   | A     | 80  | ARG  | CB-CG-CD   | -8.85  | 90.95       | 111.30   |
| 1   | B     | 182 | GLN  | OE1-CD-NE2 | -8.70  | 113.91      | 122.60   |
| 1   | D     | 143 | ASN  | OD1-CG-ND2 | 8.58   | 131.18      | 122.60   |
| 1   | A     | 53  | GLU  | CA-CB-CG   | -8.46  | 97.17       | 114.10   |
| 1   | C     | 166 | HIS  | CB-CG-CD2  | -8.46  | 120.20      | 131.20   |
| 1   | D     | 166 | HIS  | CB-CG-CD2  | -8.32  | 120.39      | 131.20   |
| 1   | A     | 143 | ASN  | OD1-CG-ND2 | 8.27   | 130.87      | 122.60   |
| 1   | C     | 182 | GLN  | OE1-CD-NE2 | -8.25  | 114.35      | 122.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 185 | PRO  | O-C-N      | 8.25  | 133.01      | 123.03   |
| 1   | D     | 182 | GLN  | OE1-CD-NE2 | -8.23 | 114.37      | 122.60   |
| 1   | A     | 182 | GLN  | OE1-CD-NE2 | -8.18 | 114.42      | 122.60   |
| 1   | D     | 80  | ARG  | CB-CG-CD   | -8.16 | 92.53       | 111.30   |
| 1   | D     | 201 | GLU  | CA-C-O     | -8.15 | 111.78      | 120.42   |
| 1   | A     | 197 | LYS  | CB-CG-CD   | -8.09 | 92.69       | 111.30   |
| 1   | C     | 178 | ILE  | CA-C-N     | 8.08  | 128.91      | 119.94   |
| 1   | C     | 178 | ILE  | C-N-CA     | 8.08  | 128.91      | 119.94   |
| 1   | B     | 53  | GLU  | CA-CB-CG   | -8.04 | 98.01       | 114.10   |
| 1   | A     | 201 | GLU  | CA-C-O     | -8.02 | 112.05      | 120.55   |
| 1   | C     | 53  | GLU  | CA-CB-CG   | -8.00 | 98.09       | 114.10   |
| 1   | D     | 53  | GLU  | CA-CB-CG   | -7.89 | 98.31       | 114.10   |
| 1   | D     | 24  | LYS  | CA-CB-CG   | -7.85 | 98.41       | 114.10   |
| 1   | B     | 92  | ASP  | CA-CB-CG   | 7.84  | 120.44      | 112.60   |
| 1   | D     | 197 | LYS  | CB-CG-CD   | -7.83 | 93.30       | 111.30   |
| 1   | D     | 184 | PRO  | O-C-N      | -7.78 | 117.50      | 121.15   |
| 1   | B     | 197 | LYS  | CB-CG-CD   | -7.75 | 93.47       | 111.30   |
| 1   | B     | 166 | HIS  | CB-CG-CD2  | -7.73 | 121.15      | 131.20   |
| 1   | A     | 25  | ASP  | CA-CB-CG   | 7.72  | 120.32      | 112.60   |
| 1   | D     | 114 | THR  | CA-CB-OG1  | 7.72  | 121.18      | 109.60   |
| 1   | C     | 114 | THR  | CA-CB-OG1  | 7.57  | 120.95      | 109.60   |
| 1   | A     | 185 | PRO  | O-C-N      | 7.56  | 132.18      | 123.03   |
| 1   | C     | 197 | LYS  | CB-CG-CD   | -7.52 | 94.00       | 111.30   |
| 1   | A     | 77  | SER  | CA-C-O     | 7.45  | 128.52      | 120.32   |
| 1   | D     | 25  | ASP  | CA-CB-CG   | 7.43  | 120.03      | 112.60   |
| 1   | D     | 92  | ASP  | CA-CB-CG   | 7.43  | 120.03      | 112.60   |
| 1   | B     | 114 | THR  | CA-CB-OG1  | 7.41  | 120.71      | 109.60   |
| 1   | C     | 77  | SER  | CA-C-O     | 7.40  | 128.46      | 120.32   |
| 1   | B     | 178 | ILE  | CA-C-N     | 7.40  | 128.15      | 119.94   |
| 1   | B     | 178 | ILE  | C-N-CA     | 7.40  | 128.15      | 119.94   |
| 1   | A     | 166 | HIS  | CB-CG-CD2  | -7.39 | 121.59      | 131.20   |
| 1   | A     | 24  | LYS  | CA-CB-CG   | -7.36 | 99.38       | 114.10   |
| 1   | D     | 66  | HIS  | CB-CG-CD2  | -7.30 | 121.71      | 131.20   |
| 1   | B     | 185 | PRO  | O-C-N      | 7.28  | 131.84      | 123.03   |
| 1   | B     | 143 | ASN  | OD1-CG-ND2 | 7.27  | 129.87      | 122.60   |
| 1   | C     | 92  | ASP  | CA-CB-CG   | 7.25  | 119.85      | 112.60   |
| 1   | B     | 185 | PRO  | CA-C-O     | 7.25  | 129.60      | 121.34   |
| 1   | A     | 114 | THR  | CA-CB-OG1  | 7.25  | 120.47      | 109.60   |
| 1   | C     | 80  | ARG  | CB-CG-CD   | -7.23 | 94.67       | 111.30   |
| 1   | C     | 33  | ASP  | N-CA-C     | 7.20  | 119.13      | 111.28   |
| 1   | B     | 80  | ARG  | CB-CG-CD   | -7.19 | 94.76       | 111.30   |
| 1   | A     | 68  | GLY  | O-C-N      | 7.15  | 129.02      | 123.23   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 139 | LEU  | CA-C-O    | 7.14  | 126.69      | 119.97   |
| 1   | D     | 176 | ASP  | CA-CB-CG  | 7.14  | 119.75      | 112.60   |
| 1   | A     | 178 | ILE  | CA-C-N    | 7.14  | 127.91      | 119.98   |
| 1   | A     | 178 | ILE  | C-N-CA    | 7.14  | 127.91      | 119.98   |
| 1   | B     | 25  | ASP  | CA-CB-CG  | 7.12  | 119.72      | 112.60   |
| 1   | C     | 155 | THR  | N-CA-CB   | -7.11 | 99.61       | 110.13   |
| 1   | A     | 176 | ASP  | CA-CB-CG  | 7.10  | 119.70      | 112.60   |
| 1   | B     | 58  | GLU  | CA-CB-CG  | 7.05  | 128.21      | 114.10   |
| 1   | C     | 176 | ASP  | CA-CB-CG  | 7.04  | 119.64      | 112.60   |
| 1   | C     | 155 | THR  | CA-CB-OG1 | -7.00 | 99.11       | 109.60   |
| 1   | B     | 89  | ARG  | CB-CG-CD  | 6.98  | 127.36      | 111.30   |
| 1   | A     | 155 | THR  | N-CA-CB   | -6.97 | 99.82       | 110.13   |
| 1   | B     | 166 | HIS  | CB-CG-ND1 | 6.97  | 133.15      | 122.70   |
| 1   | C     | 153 | SER  | CA-CB-OG  | 6.93  | 124.96      | 111.10   |
| 1   | A     | 170 | ILE  | CA-C-N    | 6.92  | 127.21      | 119.32   |
| 1   | A     | 170 | ILE  | C-N-CA    | 6.92  | 127.21      | 119.32   |
| 1   | A     | 155 | THR  | CA-CB-OG1 | -6.90 | 99.25       | 109.60   |
| 1   | D     | 155 | THR  | N-CA-CB   | -6.88 | 99.94       | 110.13   |
| 1   | D     | 143 | ASN  | CB-CG-ND2 | -6.88 | 106.08      | 116.40   |
| 1   | A     | 100 | ASP  | N-CA-C    | 6.85  | 120.69      | 111.24   |
| 1   | A     | 79  | GLU  | N-CA-C    | 6.84  | 119.65      | 109.59   |
| 1   | B     | 155 | THR  | CA-CB-OG1 | -6.83 | 99.35       | 109.60   |
| 1   | D     | 185 | PRO  | CA-C-O    | 6.83  | 129.12      | 121.34   |
| 1   | B     | 24  | LYS  | CA-CB-CG  | -6.82 | 100.46      | 114.10   |
| 1   | A     | 92  | ASP  | CA-CB-CG  | 6.82  | 119.42      | 112.60   |
| 1   | C     | 24  | LYS  | CA-CB-CG  | -6.80 | 100.49      | 114.10   |
| 1   | D     | 178 | ILE  | CA-C-N    | 6.80  | 127.49      | 119.94   |
| 1   | D     | 178 | ILE  | C-N-CA    | 6.80  | 127.49      | 119.94   |
| 1   | B     | 155 | THR  | N-CA-CB   | -6.79 | 100.08      | 110.13   |
| 1   | B     | 170 | ILE  | CA-C-N    | 6.79  | 127.06      | 119.32   |
| 1   | B     | 170 | ILE  | C-N-CA    | 6.79  | 127.06      | 119.32   |
| 1   | A     | 33  | ASP  | N-CA-C    | 6.78  | 118.67      | 111.28   |
| 1   | C     | 166 | HIS  | CB-CG-ND1 | 6.75  | 132.82      | 122.70   |
| 1   | C     | 89  | ARG  | CB-CG-CD  | 6.73  | 126.78      | 111.30   |
| 1   | A     | 66  | HIS  | CB-CG-CD2 | -6.72 | 122.47      | 131.20   |
| 1   | C     | 25  | ASP  | CA-CB-CG  | 6.72  | 119.32      | 112.60   |
| 1   | D     | 100 | ASP  | N-CA-C    | 6.72  | 120.51      | 111.24   |
| 1   | B     | 65  | ILE  | CA-C-O    | 6.71  | 127.05      | 120.27   |
| 1   | C     | 100 | ASP  | N-CA-C    | 6.69  | 120.47      | 111.24   |
| 1   | B     | 155 | THR  | CA-CB-CG2 | 6.68  | 121.86      | 110.50   |
| 1   | C     | 185 | PRO  | O-C-N     | 6.68  | 131.11      | 123.03   |
| 1   | D     | 183 | VAL  | CA-C-N    | 6.67  | 124.47      | 119.66   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 183 | VAL  | C-N-CA     | 6.67  | 124.47      | 119.66   |
| 1   | B     | 5   | VAL  | CA-C-O     | 6.65  | 126.84      | 120.25   |
| 1   | D     | 155 | THR  | CA-CB-OG1  | -6.64 | 99.64       | 109.60   |
| 1   | C     | 155 | THR  | CA-CB-CG2  | 6.63  | 121.77      | 110.50   |
| 1   | B     | 117 | ILE  | N-CA-C     | 6.63  | 117.38      | 110.62   |
| 1   | D     | 89  | ARG  | CB-CG-CD   | 6.63  | 126.55      | 111.30   |
| 1   | C     | 143 | ASN  | OD1-CG-ND2 | 6.61  | 129.21      | 122.60   |
| 1   | C     | 66  | HIS  | CB-CG-CD2  | -6.60 | 122.62      | 131.20   |
| 1   | C     | 53  | GLU  | CB-CG-CD   | 6.59  | 123.80      | 112.60   |
| 1   | C     | 190 | GLU  | CB-CG-CD   | 6.58  | 123.79      | 112.60   |
| 1   | D     | 155 | THR  | CA-CB-CG2  | 6.58  | 121.68      | 110.50   |
| 1   | A     | 89  | ARG  | CB-CG-CD   | 6.57  | 126.41      | 111.30   |
| 1   | B     | 190 | GLU  | CB-CG-CD   | 6.56  | 123.76      | 112.60   |
| 1   | C     | 207 | LEU  | O-C-N      | 6.54  | 131.13      | 122.56   |
| 1   | A     | 190 | GLU  | CB-CG-CD   | 6.54  | 123.71      | 112.60   |
| 1   | B     | 153 | SER  | CA-CB-OG   | 6.50  | 124.11      | 111.10   |
| 1   | D     | 77  | SER  | CA-C-O     | 6.50  | 127.47      | 120.32   |
| 1   | C     | 99  | GLU  | CB-CG-CD   | 6.50  | 123.65      | 112.60   |
| 1   | D     | 33  | ASP  | N-CA-C     | 6.48  | 118.34      | 111.28   |
| 1   | C     | 117 | ILE  | N-CA-C     | 6.47  | 119.14      | 111.05   |
| 1   | A     | 99  | GLU  | CB-CG-CD   | 6.47  | 123.60      | 112.60   |
| 1   | C     | 73  | ARG  | NE-CZ-NH1  | 6.47  | 127.97      | 121.50   |
| 1   | C     | 185 | PRO  | CA-C-O     | 6.46  | 128.71      | 121.34   |
| 1   | A     | 185 | PRO  | CA-C-O     | 6.46  | 128.70      | 121.34   |
| 1   | D     | 135 | ASN  | OD1-CG-ND2 | -6.45 | 116.15      | 122.60   |
| 1   | D     | 153 | SER  | CA-CB-OG   | 6.45  | 123.99      | 111.10   |
| 1   | A     | 5   | VAL  | CA-C-O     | 6.44  | 126.63      | 120.25   |
| 1   | C     | 58  | GLU  | CA-CB-CG   | 6.44  | 126.99      | 114.10   |
| 1   | D     | 166 | HIS  | CB-CG-ND1  | 6.43  | 132.35      | 122.70   |
| 1   | B     | 66  | HIS  | CB-CG-CD2  | -6.42 | 122.85      | 131.20   |
| 1   | B     | 146 | MET  | CG-SD-CE   | 6.42  | 115.02      | 100.90   |
| 1   | D     | 99  | GLU  | CB-CG-CD   | 6.40  | 123.49      | 112.60   |
| 1   | D     | 190 | GLU  | CB-CG-CD   | 6.39  | 123.47      | 112.60   |
| 1   | A     | 153 | SER  | CA-CB-OG   | 6.38  | 123.86      | 111.10   |
| 1   | C     | 141 | LEU  | N-CA-C     | 6.37  | 119.04      | 111.71   |
| 1   | C     | 65  | ILE  | CA-C-O     | 6.36  | 126.69      | 120.27   |
| 1   | D     | 79  | GLU  | N-CA-C     | 6.35  | 118.92      | 109.59   |
| 1   | B     | 172 | GLU  | CA-CB-CG   | 6.33  | 126.76      | 114.10   |
| 1   | D     | 58  | GLU  | CA-CB-CG   | 6.33  | 126.75      | 114.10   |
| 1   | A     | 5   | VAL  | N-CA-C     | -6.32 | 98.37       | 107.78   |
| 1   | C     | 14  | GLU  | N-CA-C     | -6.31 | 100.23      | 110.20   |
| 1   | A     | 58  | GLU  | CA-CB-CG   | 6.29  | 126.69      | 114.10   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 207 | LEU  | O-C-N      | 6.29  | 130.80      | 122.56   |
| 1   | B     | 99  | GLU  | CB-CG-CD   | 6.28  | 123.28      | 112.60   |
| 1   | D     | 119 | LYS  | N-CA-C     | -6.27 | 104.53      | 111.36   |
| 1   | C     | 148 | LEU  | N-CA-C     | 6.25  | 119.75      | 111.75   |
| 1   | A     | 155 | THR  | CA-CB-CG2  | 6.24  | 121.12      | 110.50   |
| 1   | A     | 207 | LEU  | O-C-N      | 6.20  | 130.68      | 122.56   |
| 1   | B     | 79  | GLU  | N-CA-C     | 6.19  | 119.24      | 109.96   |
| 1   | A     | 53  | GLU  | CB-CG-CD   | 6.16  | 123.07      | 112.60   |
| 1   | A     | 73  | ARG  | NE-CZ-NH1  | 6.15  | 127.65      | 121.50   |
| 1   | C     | 139 | LEU  | CA-C-O     | 6.15  | 127.59      | 121.20   |
| 1   | B     | 77  | SER  | CA-C-O     | 6.12  | 127.06      | 120.32   |
| 1   | B     | 80  | ARG  | NE-CZ-NH2  | -6.12 | 113.69      | 119.20   |
| 1   | B     | 176 | ASP  | CA-CB-CG   | 6.11  | 118.70      | 112.60   |
| 1   | C     | 32  | GLY  | CA-C-N     | 6.10  | 128.46      | 120.28   |
| 1   | C     | 32  | GLY  | C-N-CA     | 6.10  | 128.46      | 120.28   |
| 1   | C     | 172 | GLU  | CA-CB-CG   | 6.10  | 126.30      | 114.10   |
| 1   | C     | 197 | LYS  | CA-C-O     | -6.10 | 113.96      | 120.42   |
| 1   | B     | 33  | ASP  | N-CA-C     | 6.08  | 118.70      | 111.71   |
| 1   | D     | 65  | ILE  | CA-C-O     | 6.08  | 126.41      | 120.27   |
| 1   | C     | 172 | GLU  | CB-CG-CD   | 6.04  | 122.86      | 112.60   |
| 1   | B     | 14  | GLU  | N-CA-C     | -6.04 | 100.67      | 110.20   |
| 1   | A     | 172 | GLU  | CB-CG-CD   | 6.03  | 122.85      | 112.60   |
| 1   | C     | 93  | ASN  | OD1-CG-ND2 | -6.03 | 116.58      | 122.60   |
| 1   | B     | 100 | ASP  | N-CA-C     | 6.00  | 119.52      | 111.24   |
| 1   | B     | 24  | LYS  | N-CA-C     | 6.00  | 118.78      | 111.82   |
| 1   | D     | 14  | GLU  | N-CA-C     | -5.99 | 100.73      | 110.20   |
| 1   | D     | 114 | THR  | CA-CB-CG2  | -5.99 | 100.32      | 110.50   |
| 1   | B     | 81  | ILE  | N-CA-C     | 5.99  | 116.91      | 108.17   |
| 1   | D     | 148 | LEU  | N-CA-C     | 5.98  | 119.41      | 111.75   |
| 1   | B     | 22  | ILE  | CA-C-N     | 5.98  | 128.29      | 120.28   |
| 1   | B     | 22  | ILE  | C-N-CA     | 5.98  | 128.29      | 120.28   |
| 1   | D     | 32  | GLY  | CA-C-N     | 5.98  | 128.29      | 120.28   |
| 1   | D     | 32  | GLY  | C-N-CA     | 5.98  | 128.29      | 120.28   |
| 1   | D     | 170 | ILE  | CA-C-N     | 5.98  | 126.13      | 119.32   |
| 1   | D     | 170 | ILE  | C-N-CA     | 5.98  | 126.13      | 119.32   |
| 1   | A     | 114 | THR  | CA-CB-CG2  | -5.96 | 100.38      | 110.50   |
| 1   | A     | 141 | LEU  | N-CA-C     | 5.95  | 118.55      | 111.71   |
| 1   | B     | 53  | GLU  | CB-CG-CD   | 5.94  | 122.70      | 112.60   |
| 1   | B     | 93  | ASN  | OD1-CG-ND2 | -5.92 | 116.68      | 122.60   |
| 1   | D     | 68  | GLY  | O-C-N      | 5.92  | 129.07      | 123.57   |
| 1   | A     | 111 | TYR  | CA-C-O     | 5.92  | 126.89      | 120.32   |
| 1   | C     | 149 | SER  | CA-CB-OG   | 5.92  | 122.93      | 111.10   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 135 | ASN  | OD1-CG-ND2 | -5.91 | 116.69      | 122.60   |
| 1   | C     | 79  | GLU  | N-CA-C     | 5.89  | 118.80      | 109.96   |
| 1   | D     | 111 | TYR  | CA-C-O     | 5.88  | 126.85      | 120.32   |
| 1   | C     | 135 | ASN  | OD1-CG-ND2 | -5.88 | 116.72      | 122.60   |
| 1   | D     | 172 | GLU  | CA-CB-CG   | 5.88  | 125.86      | 114.10   |
| 1   | D     | 53  | GLU  | CB-CG-CD   | 5.86  | 122.56      | 112.60   |
| 1   | C     | 170 | ILE  | CA-C-N     | 5.85  | 125.99      | 119.32   |
| 1   | C     | 170 | ILE  | C-N-CA     | 5.85  | 125.99      | 119.32   |
| 1   | C     | 177 | LYS  | CA-C-N     | 5.84  | 128.76      | 120.53   |
| 1   | C     | 177 | LYS  | C-N-CA     | 5.84  | 128.76      | 120.53   |
| 1   | A     | 139 | LEU  | CA-C-O     | 5.82  | 126.26      | 121.02   |
| 1   | B     | 141 | LEU  | N-CA-C     | 5.79  | 118.37      | 111.71   |
| 1   | C     | 197 | LYS  | CB-CA-C    | -5.79 | 101.01      | 110.85   |
| 1   | D     | 73  | ARG  | NE-CZ-NH1  | 5.79  | 127.28      | 121.50   |
| 1   | A     | 117 | ILE  | N-CA-C     | 5.78  | 118.28      | 111.05   |
| 1   | D     | 93  | ASN  | OD1-CG-ND2 | -5.78 | 116.82      | 122.60   |
| 1   | A     | 65  | ILE  | CA-C-O     | 5.77  | 126.09      | 120.27   |
| 1   | A     | 93  | ASN  | OD1-CG-ND2 | -5.76 | 116.84      | 122.60   |
| 1   | B     | 73  | ARG  | NE-CZ-NH1  | 5.75  | 127.25      | 121.50   |
| 1   | B     | 172 | GLU  | CB-CG-CD   | 5.74  | 122.36      | 112.60   |
| 1   | D     | 172 | GLU  | CB-CG-CD   | 5.74  | 122.36      | 112.60   |
| 1   | D     | 5   | VAL  | N-CA-C     | -5.74 | 99.79       | 108.17   |
| 1   | B     | 114 | THR  | CA-CB-CG2  | -5.73 | 100.76      | 110.50   |
| 1   | D     | 141 | LEU  | N-CA-C     | 5.72  | 118.28      | 111.71   |
| 1   | B     | 32  | GLY  | CA-C-N     | 5.71  | 128.50      | 120.28   |
| 1   | B     | 32  | GLY  | C-N-CA     | 5.71  | 128.50      | 120.28   |
| 1   | B     | 207 | LEU  | O-C-N      | 5.70  | 130.03      | 122.56   |
| 1   | B     | 197 | LYS  | CA-C-O     | -5.67 | 114.41      | 120.42   |
| 1   | A     | 14  | GLU  | N-CA-C     | -5.65 | 101.27      | 110.20   |
| 1   | A     | 32  | GLY  | CA-C-N     | 5.64  | 127.84      | 120.28   |
| 1   | A     | 32  | GLY  | C-N-CA     | 5.64  | 127.84      | 120.28   |
| 1   | C     | 125 | HIS  | CB-CG-CD2  | -5.63 | 123.88      | 131.20   |
| 1   | A     | 172 | GLU  | CA-CB-CG   | 5.62  | 125.35      | 114.10   |
| 1   | A     | 70  | ALA  | CA-C-N     | 5.62  | 126.86      | 119.84   |
| 1   | A     | 70  | ALA  | C-N-CA     | 5.62  | 126.86      | 119.84   |
| 1   | C     | 143 | ASN  | CB-CG-ND2  | -5.62 | 107.97      | 116.40   |
| 1   | A     | 35  | GLN  | CB-CG-CD   | 5.62  | 122.15      | 112.60   |
| 1   | A     | 197 | LYS  | CB-CA-C    | -5.62 | 101.30      | 110.85   |
| 1   | A     | 97  | LYS  | N-CA-C     | -5.61 | 99.58       | 108.73   |
| 1   | B     | 143 | ASN  | CB-CG-ND2  | -5.61 | 107.98      | 116.40   |
| 1   | C     | 22  | ILE  | CA-C-N     | 5.61  | 127.80      | 120.28   |
| 1   | C     | 22  | ILE  | C-N-CA     | 5.61  | 127.80      | 120.28   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | C     | 141 | LEU  | CA-C-O    | -5.59 | 113.78      | 120.10   |
| 1   | B     | 70  | ALA  | CA-C-N    | 5.59  | 126.83      | 119.84   |
| 1   | B     | 70  | ALA  | C-N-CA    | 5.59  | 126.83      | 119.84   |
| 1   | A     | 149 | SER  | CA-CB-OG  | 5.58  | 122.25      | 111.10   |
| 1   | B     | 148 | LEU  | N-CA-C    | 5.57  | 118.07      | 111.33   |
| 1   | C     | 114 | THR  | CA-CB-CG2 | -5.57 | 101.03      | 110.50   |
| 1   | D     | 81  | ILE  | CB-CA-C   | -5.57 | 101.48      | 110.28   |
| 1   | C     | 35  | GLN  | CB-CG-CD  | 5.56  | 122.05      | 112.60   |
| 1   | B     | 140 | TYR  | CA-C-N    | 5.55  | 128.27      | 120.28   |
| 1   | B     | 140 | TYR  | C-N-CA    | 5.55  | 128.27      | 120.28   |
| 1   | C     | 80  | ARG  | NE-CZ-NH2 | -5.55 | 114.21      | 119.20   |
| 1   | B     | 97  | LYS  | N-CA-C    | -5.54 | 99.71       | 108.73   |
| 1   | A     | 165 | ILE  | CA-C-O    | 5.53  | 126.19      | 120.39   |
| 1   | C     | 81  | ILE  | N-CA-C    | 5.51  | 116.22      | 108.17   |
| 1   | A     | 22  | ILE  | CA-C-N    | 5.51  | 127.60      | 120.44   |
| 1   | A     | 22  | ILE  | C-N-CA    | 5.51  | 127.60      | 120.44   |
| 1   | D     | 45  | PHE  | CA-CB-CG  | 5.51  | 119.31      | 113.80   |
| 1   | C     | 113 | SER  | CA-CB-OG  | 5.49  | 122.08      | 111.10   |
| 1   | B     | 197 | LYS  | CB-CA-C   | -5.48 | 101.54      | 110.85   |
| 1   | A     | 144 | TYR  | CA-C-O    | -5.46 | 115.09      | 120.82   |
| 1   | A     | 154 | ALA  | N-CA-C    | 5.45  | 117.31      | 111.36   |
| 1   | C     | 154 | ALA  | CA-C-N    | 5.43  | 129.78      | 120.71   |
| 1   | C     | 154 | ALA  | C-N-CA    | 5.43  | 129.78      | 120.71   |
| 1   | A     | 119 | LYS  | N-CA-C    | -5.42 | 105.45      | 111.36   |
| 1   | C     | 166 | HIS  | CA-C-O    | 5.42  | 126.34      | 120.43   |
| 1   | D     | 32  | GLY  | O-C-N     | 5.42  | 129.75      | 122.70   |
| 1   | D     | 35  | GLN  | CB-CG-CD  | 5.42  | 121.82      | 112.60   |
| 1   | B     | 109 | THR  | N-CA-C    | -5.40 | 105.29      | 111.07   |
| 1   | D     | 113 | SER  | CA-CB-OG  | 5.39  | 121.89      | 111.10   |
| 1   | B     | 68  | GLY  | O-C-N     | 5.39  | 128.50      | 123.54   |
| 1   | A     | 151 | HIS  | CA-CB-CG  | -5.38 | 108.42      | 113.80   |
| 1   | C     | 119 | LYS  | N-CA-C    | -5.38 | 105.08      | 111.69   |
| 1   | B     | 35  | GLN  | CB-CG-CD  | 5.37  | 121.73      | 112.60   |
| 1   | C     | 197 | LYS  | N-CA-CB   | 5.37  | 118.11      | 110.16   |
| 1   | B     | 104 | VAL  | CA-C-N    | 5.36  | 126.55      | 119.84   |
| 1   | B     | 104 | VAL  | C-N-CA    | 5.36  | 126.55      | 119.84   |
| 1   | B     | 139 | LEU  | CA-C-O    | 5.36  | 125.79      | 120.32   |
| 1   | C     | 140 | TYR  | CA-C-N    | 5.36  | 127.99      | 120.28   |
| 1   | C     | 140 | TYR  | C-N-CA    | 5.36  | 127.99      | 120.28   |
| 1   | A     | 81  | ILE  | N-CA-C    | 5.35  | 115.98      | 108.17   |
| 1   | D     | 97  | LYS  | N-CA-C    | -5.34 | 100.02      | 108.73   |
| 1   | D     | 5   | VAL  | CA-C-O    | 5.33  | 126.24      | 120.43   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 146 | MET  | CG-SD-CE   | 5.33  | 112.62      | 100.90   |
| 1   | D     | 80  | ARG  | NE-CZ-NH2  | -5.29 | 114.44      | 119.20   |
| 1   | A     | 197 | LYS  | CA-C-O     | -5.29 | 114.82      | 120.42   |
| 1   | C     | 146 | MET  | CG-SD-CE   | 5.28  | 112.52      | 100.90   |
| 1   | A     | 137 | ALA  | CA-C-O     | 5.28  | 126.18      | 119.95   |
| 1   | A     | 86  | ILE  | CB-CA-C    | -5.27 | 102.76      | 110.62   |
| 1   | D     | 89  | ARG  | CA-CB-CG   | 5.26  | 124.62      | 114.10   |
| 1   | B     | 140 | TYR  | N-CA-CB    | -5.25 | 102.50      | 108.96   |
| 1   | C     | 5   | VAL  | N-CA-C     | -5.25 | 100.56      | 108.12   |
| 1   | A     | 166 | HIS  | CB-CG-ND1  | 5.25  | 130.57      | 122.70   |
| 1   | B     | 80  | ARG  | N-CA-C     | 5.24  | 118.14      | 111.69   |
| 1   | D     | 120 | ILE  | N-CA-C     | -5.23 | 105.40      | 110.42   |
| 1   | D     | 154 | ALA  | N-CA-C     | 5.23  | 117.89      | 111.82   |
| 1   | A     | 177 | LYS  | CA-C-N     | 5.23  | 127.90      | 120.53   |
| 1   | A     | 177 | LYS  | C-N-CA     | 5.23  | 127.90      | 120.53   |
| 1   | B     | 73  | ARG  | CD-NE-CZ   | 5.23  | 131.72      | 124.40   |
| 1   | B     | 81  | ILE  | CB-CA-C    | -5.22 | 102.03      | 110.28   |
| 1   | C     | 70  | ALA  | CA-C-N     | 5.21  | 126.35      | 119.84   |
| 1   | C     | 70  | ALA  | C-N-CA     | 5.21  | 126.35      | 119.84   |
| 1   | A     | 196 | VAL  | CA-C-O     | -5.20 | 114.85      | 120.47   |
| 1   | D     | 80  | ARG  | NE-CZ-NH1  | 5.20  | 126.70      | 121.50   |
| 1   | B     | 89  | ARG  | CA-CB-CG   | 5.20  | 124.49      | 114.10   |
| 1   | C     | 93  | ASN  | CB-CG-ND2  | 5.20  | 124.19      | 116.40   |
| 1   | B     | 57  | GLU  | CA-C-N     | 5.19  | 127.50      | 120.44   |
| 1   | B     | 57  | GLU  | C-N-CA     | 5.19  | 127.50      | 120.44   |
| 1   | D     | 84  | ASN  | CB-CG-ND2  | -5.18 | 108.62      | 116.40   |
| 1   | B     | 189 | TYR  | O-C-N      | 5.18  | 127.61      | 122.12   |
| 1   | D     | 183 | VAL  | CA-C-O     | 5.18  | 126.89      | 119.95   |
| 1   | B     | 113 | SER  | CA-CB-OG   | 5.18  | 121.46      | 111.10   |
| 1   | A     | 47  | LYS  | CA-CB-CG   | -5.17 | 103.75      | 114.10   |
| 1   | A     | 84  | ASN  | CB-CG-ND2  | -5.17 | 108.64      | 116.40   |
| 1   | B     | 154 | ALA  | N-CA-C     | 5.17  | 117.82      | 111.82   |
| 1   | C     | 202 | VAL  | CA-C-N     | 5.16  | 127.14      | 120.44   |
| 1   | C     | 202 | VAL  | C-N-CA     | 5.16  | 127.14      | 120.44   |
| 1   | A     | 135 | ASN  | OD1-CG-ND2 | -5.15 | 117.45      | 122.60   |
| 1   | A     | 113 | SER  | CA-CB-OG   | 5.15  | 121.40      | 111.10   |
| 1   | A     | 86  | ILE  | N-CA-C     | -5.15 | 101.07      | 108.48   |
| 1   | D     | 117 | ILE  | N-CA-C     | 5.14  | 117.48      | 111.05   |
| 1   | D     | 81  | ILE  | N-CA-C     | 5.14  | 115.67      | 108.17   |
| 1   | B     | 149 | SER  | CA-CB-OG   | 5.13  | 121.36      | 111.10   |
| 1   | C     | 47  | LYS  | CA-CB-CG   | -5.13 | 103.85      | 114.10   |
| 1   | D     | 127 | ARG  | NE-CZ-NH2  | -5.12 | 114.59      | 119.20   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 204 | LEU  | O-C-N     | -5.11 | 116.32      | 122.15   |
| 1   | C     | 84  | ASN  | CB-CG-ND2 | -5.11 | 108.73      | 116.40   |
| 1   | D     | 37  | PHE  | O-C-N     | 5.11  | 129.38      | 123.30   |
| 1   | D     | 144 | TYR  | CA-C-O    | -5.11 | 115.45      | 120.82   |
| 1   | D     | 197 | LYS  | N-CA-CB   | 5.09  | 118.18      | 110.28   |
| 1   | C     | 133 | ILE  | O-C-N     | -5.09 | 117.13      | 122.68   |
| 1   | D     | 189 | TYR  | CA-CB-CG  | -5.09 | 104.75      | 113.90   |
| 1   | C     | 53  | GLU  | CA-C-O    | -5.08 | 114.60      | 120.24   |
| 1   | B     | 183 | VAL  | CA-C-O    | 5.08  | 126.76      | 119.95   |
| 1   | C     | 108 | PRO  | N-CA-C    | 5.06  | 119.16      | 111.11   |
| 1   | A     | 93  | ASN  | N-CA-C    | 5.06  | 121.58      | 110.80   |
| 1   | D     | 197 | LYS  | CB-CA-C   | -5.06 | 100.96      | 110.67   |
| 1   | A     | 93  | ASN  | CB-CG-ND2 | 5.05  | 123.98      | 116.40   |
| 1   | C     | 155 | THR  | CB-CA-C   | 5.05  | 119.27      | 110.79   |
| 1   | D     | 22  | ILE  | CA-C-N    | 5.04  | 127.00      | 120.44   |
| 1   | D     | 22  | ILE  | C-N-CA    | 5.04  | 127.00      | 120.44   |
| 1   | C     | 89  | ARG  | CA-CB-CG  | 5.03  | 124.16      | 114.10   |
| 1   | C     | 152 | HIS  | CB-CG-CD2 | -5.03 | 124.66      | 131.20   |
| 1   | C     | 154 | ALA  | N-CA-C    | 5.03  | 116.84      | 111.36   |
| 1   | B     | 45  | PHE  | CA-CB-CG  | 5.01  | 118.81      | 113.80   |
| 1   | D     | 50  | GLU  | N-CA-CB   | -5.01 | 102.59      | 109.91   |
| 1   | C     | 45  | PHE  | CA-CB-CG  | 5.01  | 118.81      | 113.80   |
| 1   | B     | 197 | LYS  | N-CA-CB   | 5.01  | 117.57      | 110.16   |
| 1   | B     | 119 | LYS  | N-CA-C    | -5.00 | 105.91      | 111.36   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 144 | TYR  | Sidechain |
| 1   | B     | 189 | TYR  | Sidechain |
| 1   | D     | 144 | TYR  | 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     | 1605  | 0        | 1671     | 75      | 0            |
| 1   | B     | 1605  | 0        | 1671     | 69      | 0            |
| 1   | C     | 1605  | 0        | 1671     | 68      | 0            |
| 1   | D     | 1605  | 0        | 1671     | 73      | 0            |
| 2   | A     | 30    | 0        | 0        | 3       | 0            |
| 2   | B     | 34    | 0        | 0        | 0       | 0            |
| 2   | C     | 28    | 0        | 0        | 0       | 0            |
| 2   | D     | 32    | 0        | 0        | 3       | 0            |
| All | All   | 6544  | 0        | 6684     | 270     | 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 21.

All (270) 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:65:ILE:HD12  | 1:C:115:LEU:HD11 | 1.27                     | 1.16              |
| 1:A:65:ILE:HD12  | 1:A:115:LEU:HD11 | 1.29                     | 1.14              |
| 1:D:129:ILE:HD12 | 1:D:191:MET:HE2  | 1.16                     | 1.13              |
| 1:A:64:ALA:O     | 1:A:65:ILE:HD13  | 1.62                     | 0.99              |
| 1:C:64:ALA:O     | 1:C:65:ILE:HD13  | 1.62                     | 0.99              |
| 1:A:65:ILE:HD12  | 1:A:115:LEU:CD1  | 2.03                     | 0.88              |
| 1:D:175:ILE:HA   | 1:D:178:ILE:HD12 | 1.56                     | 0.88              |
| 1:C:175:ILE:HA   | 1:C:178:ILE:HD12 | 1.57                     | 0.87              |
| 1:C:116:PRO:HB2  | 1:C:119:LYS:HD2  | 1.56                     | 0.87              |
| 1:B:175:ILE:HA   | 1:B:178:ILE:HD12 | 1.57                     | 0.87              |
| 1:C:90:ILE:HD13  | 1:C:90:ILE:H     | 1.39                     | 0.87              |
| 1:A:90:ILE:H     | 1:A:90:ILE:HD13  | 1.40                     | 0.87              |
| 1:C:65:ILE:HD12  | 1:C:115:LEU:CD1  | 2.05                     | 0.86              |
| 1:B:90:ILE:HD13  | 1:B:90:ILE:H     | 1.41                     | 0.86              |
| 1:D:116:PRO:HB2  | 1:D:119:LYS:HD2  | 1.56                     | 0.85              |
| 1:B:76:ILE:HD12  | 1:B:129:ILE:CG2  | 2.06                     | 0.85              |
| 1:A:116:PRO:HB2  | 1:A:119:LYS:HD2  | 1.57                     | 0.84              |
| 1:C:103:ILE:HD12 | 1:C:144:TYR:HD1  | 1.44                     | 0.83              |
| 1:A:76:ILE:HD12  | 1:A:129:ILE:CG2  | 2.09                     | 0.83              |
| 1:B:171:PRO:HA   | 1:B:174:ILE:HD13 | 1.58                     | 0.83              |
| 1:D:70:ALA:HB1   | 1:D:73:ARG:HD3   | 1.59                     | 0.83              |
| 1:B:116:PRO:HB2  | 1:B:119:LYS:HD2  | 1.60                     | 0.82              |
| 1:C:70:ALA:HB1   | 1:C:73:ARG:HD3   | 1.62                     | 0.81              |
| 1:A:175:ILE:HA   | 1:A:178:ILE:HD12 | 1.61                     | 0.81              |
| 1:A:70:ALA:HB1   | 1:A:73:ARG:HD3   | 1.62                     | 0.81              |
| 1:A:65:ILE:CD1   | 1:A:115:LEU:HD11 | 2.09                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:76:ILE:HD12  | 1:B:129:ILE:HG22 | 1.64                     | 0.78              |
| 1:B:76:ILE:HD13  | 1:B:195:ALA:CB   | 2.16                     | 0.76              |
| 1:B:70:ALA:HB1   | 1:B:73:ARG:HD3   | 1.67                     | 0.76              |
| 1:A:76:ILE:HD13  | 1:A:195:ALA:CB   | 2.15                     | 0.75              |
| 1:A:65:ILE:HD11  | 1:A:115:LEU:CD2  | 2.17                     | 0.75              |
| 1:C:65:ILE:CD1   | 1:C:115:LEU:HD11 | 2.14                     | 0.74              |
| 1:C:65:ILE:HD11  | 1:C:115:LEU:HD21 | 1.68                     | 0.74              |
| 1:A:65:ILE:HD11  | 1:A:115:LEU:HD21 | 1.67                     | 0.74              |
| 1:C:65:ILE:HD11  | 1:C:115:LEU:CD2  | 2.20                     | 0.71              |
| 1:B:174:ILE:HD12 | 1:B:174:ILE:N    | 2.06                     | 0.71              |
| 1:C:64:ALA:C     | 1:C:65:ILE:HD13  | 2.17                     | 0.70              |
| 1:A:76:ILE:HD12  | 1:A:129:ILE:HG22 | 1.74                     | 0.69              |
| 1:B:81:ILE:HD13  | 1:C:83:VAL:HG11  | 1.73                     | 0.69              |
| 1:A:170:ILE:HD13 | 1:A:173:GLN:OE1  | 1.94                     | 0.68              |
| 1:A:56:LEU:HD22  | 1:A:159:PRO:HD3  | 1.76                     | 0.68              |
| 1:C:103:ILE:HD12 | 1:C:144:TYR:CD1  | 2.30                     | 0.67              |
| 1:D:6:THR:HA     | 1:D:39:ARG:O     | 1.95                     | 0.67              |
| 1:B:83:VAL:HG11  | 1:C:81:ILE:HD13  | 1.78                     | 0.66              |
| 1:B:76:ILE:HD13  | 1:B:195:ALA:HB1  | 1.76                     | 0.65              |
| 1:A:76:ILE:HD13  | 1:A:195:ALA:HB1  | 1.77                     | 0.64              |
| 1:B:104:VAL:HB   | 1:B:107:ALA:CB   | 2.28                     | 0.64              |
| 1:A:104:VAL:HB   | 1:A:107:ALA:HB3  | 1.80                     | 0.64              |
| 1:B:174:ILE:HD11 | 1:B:186:SER:HB3  | 1.79                     | 0.64              |
| 1:B:104:VAL:HB   | 1:B:107:ALA:HB3  | 1.79                     | 0.64              |
| 1:B:174:ILE:CD1  | 1:B:186:SER:HB3  | 2.27                     | 0.64              |
| 1:A:64:ALA:C     | 1:A:65:ILE:HD13  | 2.22                     | 0.64              |
| 1:D:78:ILE:HD13  | 1:D:165:ILE:HG12 | 1.78                     | 0.63              |
| 1:D:117:ILE:H    | 1:D:117:ILE:HD13 | 1.63                     | 0.63              |
| 1:A:104:VAL:HB   | 1:A:107:ALA:CB   | 2.29                     | 0.63              |
| 1:D:56:LEU:HD22  | 1:D:159:PRO:HD3  | 1.81                     | 0.63              |
| 1:D:49:LYS:HG3   | 1:D:148:LEU:HD13 | 1.79                     | 0.63              |
| 1:A:81:ILE:HD13  | 1:D:83:VAL:HG11  | 1.81                     | 0.63              |
| 1:A:6:THR:HA     | 1:A:39:ARG:O     | 1.99                     | 0.62              |
| 1:D:161:MET:HE1  | 1:D:206:GLU:HB3  | 1.80                     | 0.62              |
| 1:C:6:THR:HA     | 1:C:39:ARG:O     | 2.00                     | 0.62              |
| 1:B:49:LYS:HG3   | 1:B:148:LEU:HD13 | 1.82                     | 0.61              |
| 1:C:56:LEU:HD22  | 1:C:159:PRO:HD3  | 1.81                     | 0.61              |
| 1:B:6:THR:HA     | 1:B:39:ARG:O     | 1.99                     | 0.61              |
| 1:C:104:VAL:HB   | 1:C:107:ALA:HB3  | 1.83                     | 0.61              |
| 1:A:49:LYS:HG3   | 1:A:148:LEU:HD13 | 1.82                     | 0.61              |
| 1:B:56:LEU:HD22  | 1:B:159:PRO:HD3  | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:104:VAL:HB   | 1:C:107:ALA:CB   | 2.32                     | 0.60              |
| 1:D:104:VAL:HB   | 1:D:107:ALA:HB3  | 1.82                     | 0.60              |
| 1:C:117:ILE:HD13 | 1:C:117:ILE:H    | 1.65                     | 0.60              |
| 1:D:104:VAL:HB   | 1:D:107:ALA:CB   | 2.32                     | 0.60              |
| 1:C:65:ILE:CD1   | 1:C:115:LEU:HD21 | 2.30                     | 0.60              |
| 1:C:78:ILE:HD13  | 1:C:165:ILE:HG12 | 1.84                     | 0.60              |
| 1:B:76:ILE:CD1   | 1:B:129:ILE:CG2  | 2.78                     | 0.59              |
| 1:A:161:MET:HE1  | 1:A:206:GLU:HB3  | 1.83                     | 0.59              |
| 1:D:45:PHE:CE2   | 1:D:86:ILE:HD12  | 2.37                     | 0.59              |
| 1:C:161:MET:HE1  | 1:C:206:GLU:HB3  | 1.83                     | 0.59              |
| 1:C:90:ILE:H     | 1:C:90:ILE:CD1   | 2.14                     | 0.59              |
| 1:B:161:MET:HE1  | 1:B:206:GLU:HB3  | 1.83                     | 0.59              |
| 1:C:49:LYS:HG3   | 1:C:148:LEU:HD13 | 1.85                     | 0.59              |
| 1:B:115:LEU:HD23 | 1:B:161:MET:HB3  | 1.85                     | 0.58              |
| 1:D:146:MET:HG3  | 1:D:164:PHE:HB2  | 1.85                     | 0.58              |
| 1:D:80:ARG:HB3   | 1:D:81:ILE:HD13  | 1.84                     | 0.58              |
| 1:A:18:PRO:HB3   | 1:A:170:ILE:HD12 | 1.86                     | 0.58              |
| 1:B:170:ILE:O    | 1:B:174:ILE:CD1  | 2.52                     | 0.57              |
| 1:A:115:LEU:HD23 | 1:A:161:MET:HB3  | 1.86                     | 0.57              |
| 1:D:16:ILE:HD12  | 2:D:211:HOH:O    | 2.04                     | 0.57              |
| 1:D:45:PHE:HE2   | 1:D:86:ILE:HD12  | 1.68                     | 0.57              |
| 1:C:16:ILE:HD13  | 1:C:17:ASN:N     | 2.20                     | 0.56              |
| 1:A:65:ILE:CD1   | 1:A:115:LEU:HD21 | 2.33                     | 0.56              |
| 1:D:115:LEU:HD23 | 1:D:161:MET:HB3  | 1.86                     | 0.56              |
| 1:A:62:ASP:HB3   | 1:A:207:LEU:HD11 | 1.87                     | 0.56              |
| 1:C:174:ILE:HG13 | 1:C:186:SER:HB3  | 1.87                     | 0.56              |
| 1:D:78:ILE:CD1   | 1:D:165:ILE:HG12 | 2.34                     | 0.56              |
| 1:D:174:ILE:HG13 | 1:D:186:SER:HB3  | 1.88                     | 0.56              |
| 1:D:1:MET:HE1    | 1:D:207:LEU:O    | 2.06                     | 0.56              |
| 1:D:22:ILE:HG21  | 1:D:196:VAL:HG11 | 1.88                     | 0.56              |
| 1:D:11:PHE:HA    | 1:D:93:ASN:HD21  | 1.70                     | 0.56              |
| 1:C:11:PHE:HA    | 1:C:93:ASN:HD21  | 1.70                     | 0.55              |
| 1:C:78:ILE:CD1   | 1:C:165:ILE:HG12 | 2.35                     | 0.55              |
| 1:A:76:ILE:HD12  | 1:A:129:ILE:HG21 | 1.88                     | 0.55              |
| 1:C:115:LEU:HD23 | 1:C:161:MET:HB3  | 1.88                     | 0.55              |
| 1:B:76:ILE:CD1   | 1:B:129:ILE:HG21 | 2.37                     | 0.55              |
| 1:B:130:PRO:HA   | 1:D:175:ILE:HG22 | 1.88                     | 0.55              |
| 1:A:11:PHE:HA    | 1:A:93:ASN:HD21  | 1.71                     | 0.55              |
| 1:B:11:PHE:HA    | 1:B:93:ASN:HD21  | 1.70                     | 0.55              |
| 1:D:129:ILE:N    | 1:D:129:ILE:HD13 | 2.23                     | 0.54              |
| 1:B:22:ILE:HG21  | 1:B:196:VAL:HG11 | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:3:VAL:HG11   | 1:A:200:ILE:HD12 | 1.90                     | 0.54              |
| 1:B:194:GLU:O    | 1:B:198:VAL:HG23 | 2.08                     | 0.53              |
| 1:B:174:ILE:HD12 | 1:B:174:ILE:H    | 1.73                     | 0.53              |
| 1:B:174:ILE:N    | 1:B:174:ILE:CD1  | 2.71                     | 0.53              |
| 1:B:171:PRO:CA   | 1:B:174:ILE:HD13 | 2.33                     | 0.53              |
| 1:C:182:GLN:HA   | 1:C:182:GLN:NE2  | 2.24                     | 0.53              |
| 1:D:86:ILE:HG21  | 1:D:98:ILE:HB    | 1.91                     | 0.53              |
| 1:A:65:ILE:CD1   | 1:A:115:LEU:CD1  | 2.78                     | 0.52              |
| 1:B:81:ILE:CD1   | 1:C:83:VAL:HG11  | 2.39                     | 0.52              |
| 1:C:16:ILE:HD13  | 1:C:16:ILE:C     | 2.34                     | 0.52              |
| 1:D:127:ARG:O    | 1:D:129:ILE:HD13 | 2.10                     | 0.52              |
| 1:A:1:MET:HE1    | 1:A:207:LEU:O    | 2.08                     | 0.52              |
| 1:B:1:MET:HE1    | 1:B:207:LEU:O    | 2.09                     | 0.52              |
| 1:A:76:ILE:CD1   | 1:A:129:ILE:CG2  | 2.84                     | 0.52              |
| 1:B:90:ILE:H     | 1:B:90:ILE:CD1   | 2.17                     | 0.52              |
| 1:C:146:MET:HG3  | 1:C:164:PHE:HB2  | 1.91                     | 0.52              |
| 1:A:76:ILE:CD1   | 1:A:129:ILE:HG21 | 2.41                     | 0.51              |
| 1:A:22:ILE:HG21  | 1:A:196:VAL:HG11 | 1.92                     | 0.51              |
| 1:A:194:GLU:O    | 1:A:198:VAL:HG23 | 2.10                     | 0.51              |
| 1:C:86:ILE:HG13  | 1:C:103:ILE:CD1  | 2.39                     | 0.51              |
| 1:B:76:ILE:CD1   | 1:B:195:ALA:CB   | 2.88                     | 0.51              |
| 1:D:152:HIS:HD2  | 1:D:158:TYR:O    | 1.93                     | 0.51              |
| 1:A:182:GLN:HA   | 1:A:182:GLN:NE2  | 2.25                     | 0.51              |
| 1:C:39:ARG:NH2   | 1:C:59:ILE:HD11  | 2.25                     | 0.51              |
| 1:D:33:ASP:HA    | 2:D:216:HOH:O    | 2.10                     | 0.51              |
| 1:D:182:GLN:NE2  | 1:D:182:GLN:HA   | 2.26                     | 0.51              |
| 1:B:164:PHE:C    | 1:B:165:ILE:HD12 | 2.35                     | 0.51              |
| 1:A:152:HIS:HD2  | 1:A:158:TYR:O    | 1.92                     | 0.51              |
| 1:B:16:ILE:CD1   | 1:B:18:PRO:HD3   | 2.40                     | 0.51              |
| 1:A:90:ILE:H     | 1:A:90:ILE:CD1   | 2.16                     | 0.51              |
| 1:C:1:MET:HE1    | 1:C:207:LEU:O    | 2.09                     | 0.50              |
| 1:C:22:ILE:HG21  | 1:C:196:VAL:HG11 | 1.93                     | 0.50              |
| 1:B:146:MET:HG3  | 1:B:164:PHE:HB2  | 1.93                     | 0.50              |
| 1:C:152:HIS:HD2  | 1:C:158:TYR:O    | 1.94                     | 0.50              |
| 1:D:194:GLU:O    | 1:D:198:VAL:HG23 | 2.11                     | 0.50              |
| 1:B:37:PHE:CE2   | 1:B:59:ILE:HD12  | 2.47                     | 0.50              |
| 1:B:16:ILE:C     | 1:B:16:ILE:HD13  | 2.37                     | 0.50              |
| 1:A:39:ARG:NH2   | 1:A:59:ILE:HD11  | 2.27                     | 0.50              |
| 1:A:164:PHE:C    | 1:A:165:ILE:HD12 | 2.37                     | 0.49              |
| 1:B:86:ILE:HD11  | 1:B:144:TYR:CD1  | 2.48                     | 0.49              |
| 1:A:66:HIS:HD2   | 2:A:227:HOH:O    | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:174:ILE:HG13 | 1:A:186:SER:HB3  | 1.94                     | 0.49              |
| 1:B:76:ILE:CD1   | 1:B:195:ALA:HB2  | 2.42                     | 0.49              |
| 1:B:152:HIS:HD2  | 1:B:158:TYR:O    | 1.95                     | 0.49              |
| 1:B:174:ILE:CD1  | 1:B:174:ILE:H    | 2.25                     | 0.49              |
| 1:D:70:ALA:O     | 1:D:73:ARG:HB2   | 2.12                     | 0.49              |
| 1:D:80:ARG:C     | 1:D:81:ILE:HD13  | 2.38                     | 0.49              |
| 1:C:175:ILE:C    | 1:C:175:ILE:HD12 | 2.37                     | 0.49              |
| 1:D:62:ASP:HB3   | 1:D:207:LEU:HD11 | 1.94                     | 0.49              |
| 1:A:146:MET:HG3  | 1:A:164:PHE:HB2  | 1.95                     | 0.49              |
| 1:B:182:GLN:HA   | 1:B:182:GLN:NE2  | 2.27                     | 0.49              |
| 1:C:16:ILE:CD1   | 1:C:18:PRO:HD3   | 2.43                     | 0.49              |
| 1:D:37:PHE:CE2   | 1:D:59:ILE:HD12  | 2.48                     | 0.49              |
| 1:A:86:ILE:HG21  | 1:A:98:ILE:HB    | 1.94                     | 0.49              |
| 1:B:45:PHE:HE2   | 1:B:86:ILE:HD12  | 1.78                     | 0.49              |
| 1:B:174:ILE:HG12 | 1:B:186:SER:HB3  | 1.95                     | 0.49              |
| 1:D:80:ARG:CB    | 1:D:81:ILE:HD13  | 2.43                     | 0.49              |
| 1:D:117:ILE:HD13 | 1:D:117:ILE:N    | 2.28                     | 0.48              |
| 1:D:175:ILE:HD12 | 1:D:175:ILE:C    | 2.38                     | 0.48              |
| 1:A:66:HIS:CD2   | 2:A:227:HOH:O    | 2.65                     | 0.48              |
| 1:A:76:ILE:CD1   | 1:A:195:ALA:CB   | 2.89                     | 0.48              |
| 1:B:86:ILE:HG21  | 1:B:98:ILE:HB    | 1.94                     | 0.48              |
| 1:C:117:ILE:HD13 | 1:C:117:ILE:N    | 2.27                     | 0.48              |
| 1:D:104:VAL:HG23 | 1:D:147:TYR:HE2  | 1.79                     | 0.48              |
| 1:B:62:ASP:HB3   | 1:B:207:LEU:HD11 | 1.95                     | 0.48              |
| 1:B:175:ILE:HD13 | 1:D:125:HIS:O    | 2.13                     | 0.48              |
| 1:D:86:ILE:HD13  | 1:D:103:ILE:HD11 | 1.95                     | 0.48              |
| 1:A:70:ALA:O     | 1:A:73:ARG:HB2   | 2.13                     | 0.48              |
| 1:B:175:ILE:HG22 | 1:D:130:PRO:HA   | 1.95                     | 0.48              |
| 1:A:90:ILE:HD13  | 1:A:90:ILE:N     | 2.20                     | 0.47              |
| 1:C:62:ASP:HB3   | 1:C:207:LEU:HD11 | 1.96                     | 0.47              |
| 1:B:29:ILE:C     | 1:B:29:ILE:HD12  | 2.39                     | 0.47              |
| 1:C:90:ILE:HD13  | 1:C:90:ILE:N     | 2.19                     | 0.47              |
| 1:D:86:ILE:HD11  | 1:D:144:TYR:CD1  | 2.49                     | 0.47              |
| 1:A:156:LYS:HD3  | 2:A:221:HOH:O    | 2.15                     | 0.47              |
| 1:B:83:VAL:HG11  | 1:C:81:ILE:CD1   | 2.44                     | 0.47              |
| 1:C:65:ILE:CD1   | 1:C:115:LEU:CD1  | 2.84                     | 0.47              |
| 1:D:29:ILE:HD12  | 1:D:29:ILE:C     | 2.39                     | 0.47              |
| 1:D:81:ILE:HD13  | 1:D:81:ILE:N     | 2.29                     | 0.47              |
| 1:A:174:ILE:HG23 | 1:A:184:PRO:HD2  | 1.97                     | 0.47              |
| 1:B:80:ARG:CD    | 1:B:135:ASN:ND2  | 2.78                     | 0.46              |
| 1:D:23:ALA:O     | 1:D:38:GLY:HA3   | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:29:ILE:HD12  | 1:A:29:ILE:C     | 2.40                     | 0.46              |
| 1:A:104:VAL:HG23 | 1:A:147:TYR:HE2  | 1.80                     | 0.46              |
| 1:A:116:PRO:CB   | 1:A:119:LYS:HD2  | 2.38                     | 0.46              |
| 1:B:45:PHE:CE2   | 1:B:86:ILE:HD12  | 2.50                     | 0.46              |
| 1:B:16:ILE:HD13  | 1:B:17:ASN:N     | 2.30                     | 0.46              |
| 1:D:80:ARG:CD    | 1:D:135:ASN:ND2  | 2.78                     | 0.46              |
| 1:B:16:ILE:HD13  | 1:B:18:PRO:HD3   | 1.97                     | 0.46              |
| 1:C:65:ILE:CD1   | 1:C:115:LEU:CD2  | 2.93                     | 0.45              |
| 1:A:130:PRO:HA   | 1:C:175:ILE:HG22 | 1.99                     | 0.45              |
| 1:D:76:ILE:O     | 1:D:131:ALA:HA   | 2.16                     | 0.45              |
| 1:D:170:ILE:HA   | 1:D:187:MET:O    | 2.16                     | 0.45              |
| 1:A:175:ILE:HG22 | 1:C:130:PRO:HA   | 1.98                     | 0.45              |
| 1:B:80:ARG:HD2   | 1:B:135:ASN:ND2  | 2.31                     | 0.45              |
| 1:B:174:ILE:HG23 | 1:B:184:PRO:HD2  | 1.98                     | 0.45              |
| 1:A:76:ILE:CD1   | 1:A:195:ALA:HB2  | 2.46                     | 0.45              |
| 1:B:90:ILE:HD13  | 1:B:90:ILE:N     | 2.20                     | 0.45              |
| 1:C:117:ILE:H    | 1:C:117:ILE:CD1  | 2.30                     | 0.45              |
| 1:D:85:ALA:C     | 1:D:103:ILE:HD11 | 2.41                     | 0.45              |
| 1:A:109:THR:HG23 | 1:D:112:PHE:CE1  | 2.51                     | 0.45              |
| 1:B:124:LEU:HD23 | 1:B:124:LEU:HA   | 1.79                     | 0.45              |
| 1:C:174:ILE:HG23 | 1:C:184:PRO:HD2  | 1.99                     | 0.45              |
| 1:C:70:ALA:O     | 1:C:73:ARG:HB2   | 2.17                     | 0.45              |
| 1:A:65:ILE:CD1   | 1:A:115:LEU:CD2  | 2.93                     | 0.44              |
| 1:C:194:GLU:O    | 1:C:198:VAL:HG23 | 2.17                     | 0.44              |
| 1:B:130:PRO:CA   | 1:D:175:ILE:HG22 | 2.47                     | 0.44              |
| 1:C:80:ARG:CD    | 1:C:135:ASN:ND2  | 2.80                     | 0.44              |
| 1:D:80:ARG:HD2   | 1:D:135:ASN:ND2  | 2.32                     | 0.44              |
| 1:A:5:VAL:HA     | 1:A:65:ILE:O     | 2.17                     | 0.44              |
| 1:A:70:ALA:HB2   | 1:A:166:HIS:CD2  | 2.52                     | 0.44              |
| 1:B:174:ILE:CG1  | 1:B:186:SER:HB3  | 2.47                     | 0.44              |
| 1:D:16:ILE:HA    | 2:D:211:HOH:O    | 2.18                     | 0.44              |
| 1:A:124:LEU:HD23 | 1:A:124:LEU:HA   | 1.78                     | 0.44              |
| 1:C:104:VAL:HG23 | 1:C:147:TYR:HE2  | 1.82                     | 0.44              |
| 1:C:86:ILE:HG13  | 1:C:103:ILE:HD13 | 1.98                     | 0.44              |
| 1:C:174:ILE:CG1  | 1:C:186:SER:HB3  | 2.48                     | 0.44              |
| 1:A:76:ILE:HD13  | 1:A:195:ALA:HB2  | 1.99                     | 0.44              |
| 1:D:117:ILE:H    | 1:D:117:ILE:CD1  | 2.29                     | 0.44              |
| 1:A:71:PRO:HB3   | 1:A:169:TYR:CZ   | 2.53                     | 0.43              |
| 1:A:112:PHE:CE1  | 1:D:109:THR:HG23 | 2.52                     | 0.43              |
| 1:A:81:ILE:CD1   | 1:D:83:VAL:HG11  | 2.47                     | 0.43              |
| 1:D:174:ILE:HG23 | 1:D:184:PRO:HD2  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:3:VAL:HG22   | 1:C:63:ILE:HB    | 2.00                     | 0.43              |
| 1:B:170:ILE:HA   | 1:B:187:MET:O    | 2.19                     | 0.43              |
| 1:D:5:VAL:HA     | 1:D:65:ILE:O     | 2.19                     | 0.43              |
| 1:D:116:PRO:CB   | 1:D:119:LYS:HD2  | 2.38                     | 0.43              |
| 1:C:86:ILE:HG21  | 1:C:98:ILE:HB    | 2.00                     | 0.43              |
| 1:A:80:ARG:CD    | 1:A:135:ASN:ND2  | 2.81                     | 0.43              |
| 1:B:104:VAL:HG23 | 1:B:147:TYR:HE2  | 1.83                     | 0.42              |
| 1:C:26:LEU:O     | 1:C:29:ILE:HG12  | 2.18                     | 0.42              |
| 1:C:90:ILE:CD1   | 1:C:90:ILE:N     | 2.81                     | 0.42              |
| 1:D:26:LEU:O     | 1:D:29:ILE:HG13  | 2.19                     | 0.42              |
| 1:D:67:VAL:HA    | 1:D:165:ILE:O    | 2.19                     | 0.42              |
| 1:A:175:ILE:HD13 | 1:C:125:HIS:O    | 2.19                     | 0.42              |
| 1:C:80:ARG:HD3   | 1:C:135:ASN:ND2  | 2.35                     | 0.42              |
| 1:D:70:ALA:HB2   | 1:D:166:HIS:CD2  | 2.54                     | 0.42              |
| 1:D:171:PRO:HD3  | 1:D:187:MET:O    | 2.19                     | 0.42              |
| 1:A:68:GLY:O     | 1:A:166:HIS:HA   | 2.20                     | 0.42              |
| 1:A:170:ILE:HA   | 1:A:187:MET:O    | 2.20                     | 0.42              |
| 1:A:174:ILE:CG1  | 1:A:186:SER:HB3  | 2.49                     | 0.42              |
| 1:B:70:ALA:HB2   | 1:B:166:HIS:CD2  | 2.55                     | 0.42              |
| 1:D:124:LEU:HD23 | 1:D:124:LEU:HA   | 1.81                     | 0.41              |
| 1:C:8:PHE:O      | 1:C:20:GLU:HB2   | 2.20                     | 0.41              |
| 1:D:3:VAL:HG22   | 1:D:63:ILE:HB    | 2.03                     | 0.41              |
| 1:A:80:ARG:HD3   | 1:A:135:ASN:ND2  | 2.35                     | 0.41              |
| 1:C:170:ILE:HD12 | 1:C:172:GLU:HG2  | 2.02                     | 0.41              |
| 1:D:103:ILE:HD13 | 1:D:103:ILE:N    | 2.35                     | 0.41              |
| 1:D:129:ILE:N    | 1:D:129:ILE:CD1  | 2.84                     | 0.41              |
| 1:D:82:ALA:HB1   | 1:D:147:TYR:HB2  | 2.02                     | 0.41              |
| 1:A:146:MET:O    | 1:A:146:MET:HG2  | 2.21                     | 0.41              |
| 1:A:30:LYS:HB3   | 1:A:30:LYS:HE2   | 1.90                     | 0.41              |
| 1:D:8:PHE:O      | 1:D:20:GLU:HB2   | 2.21                     | 0.41              |
| 1:D:128:GLY:C    | 1:D:129:ILE:HD13 | 2.46                     | 0.41              |
| 1:B:171:PRO:HD3  | 1:B:187:MET:O    | 2.21                     | 0.41              |
| 1:A:76:ILE:O     | 1:A:131:ALA:HA   | 2.21                     | 0.40              |
| 1:C:76:ILE:O     | 1:C:131:ALA:HA   | 2.21                     | 0.40              |
| 1:C:124:LEU:HA   | 1:C:124:LEU:HD23 | 1.81                     | 0.40              |
| 1:B:119:LYS:HE3  | 1:B:119:LYS:N    | 2.37                     | 0.40              |
| 1:B:37:PHE:HD2   | 1:B:39:ARG:HH22  | 1.69                     | 0.40              |
| 1:C:5:VAL:HA     | 1:C:65:ILE:O     | 2.22                     | 0.40              |
| 1:D:43:VAL:CG1   | 1:D:141:LEU:HD13 | 2.52                     | 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     | 206/208 (99%) | 189 (92%) | 16 (8%) | 1 (0%)   | 24          | 48  |
| 1   | B     | 206/208 (99%) | 190 (92%) | 16 (8%) | 0        | 100         | 100 |
| 1   | C     | 206/208 (99%) | 188 (91%) | 18 (9%) | 0        | 100         | 100 |
| 1   | D     | 206/208 (99%) | 189 (92%) | 17 (8%) | 0        | 100         | 100 |
| All | All   | 824/832 (99%) | 756 (92%) | 67 (8%) | 1 (0%)   | 48          | 73  |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | 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     | 174/174 (100%) | 150 (86%) | 24 (14%) | 3           | 9 |
| 1   | B     | 174/174 (100%) | 149 (86%) | 25 (14%) | 3           | 8 |
| 1   | C     | 174/174 (100%) | 150 (86%) | 24 (14%) | 3           | 9 |
| 1   | D     | 174/174 (100%) | 149 (86%) | 25 (14%) | 3           | 8 |
| All | All   | 696/696 (100%) | 598 (86%) | 98 (14%) | 3           | 9 |

All (98) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | LEU  |
| 1   | A     | 29  | ILE  |
| 1   | A     | 50  | GLU  |
| 1   | A     | 52  | LEU  |
| 1   | A     | 67  | VAL  |
| 1   | A     | 69  | LEU  |
| 1   | A     | 73  | ARG  |
| 1   | A     | 81  | ILE  |
| 1   | A     | 89  | ARG  |
| 1   | A     | 90  | ILE  |
| 1   | A     | 119 | LYS  |
| 1   | A     | 122 | LYS  |
| 1   | A     | 141 | LEU  |
| 1   | A     | 145 | VAL  |
| 1   | A     | 155 | THR  |
| 1   | A     | 160 | LYS  |
| 1   | A     | 170 | ILE  |
| 1   | A     | 172 | GLU  |
| 1   | A     | 180 | LYS  |
| 1   | A     | 182 | GLN  |
| 1   | A     | 196 | VAL  |
| 1   | A     | 202 | VAL  |
| 1   | A     | 206 | GLU  |
| 1   | A     | 207 | LEU  |
| 1   | B     | 4   | LEU  |
| 1   | B     | 16  | ILE  |
| 1   | B     | 29  | ILE  |
| 1   | B     | 50  | GLU  |
| 1   | B     | 52  | LEU  |
| 1   | B     | 67  | VAL  |
| 1   | B     | 69  | LEU  |
| 1   | B     | 73  | ARG  |
| 1   | B     | 81  | ILE  |
| 1   | B     | 89  | ARG  |
| 1   | B     | 90  | ILE  |
| 1   | B     | 119 | LYS  |
| 1   | B     | 122 | LYS  |
| 1   | B     | 141 | LEU  |
| 1   | B     | 145 | VAL  |
| 1   | B     | 155 | THR  |
| 1   | B     | 160 | LYS  |
| 1   | B     | 172 | GLU  |
| 1   | B     | 174 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 180 | LYS  |
| 1   | B     | 182 | GLN  |
| 1   | B     | 196 | VAL  |
| 1   | B     | 202 | VAL  |
| 1   | B     | 206 | GLU  |
| 1   | B     | 207 | LEU  |
| 1   | C     | 4   | LEU  |
| 1   | C     | 16  | ILE  |
| 1   | C     | 50  | GLU  |
| 1   | C     | 52  | LEU  |
| 1   | C     | 67  | VAL  |
| 1   | C     | 69  | LEU  |
| 1   | C     | 73  | ARG  |
| 1   | C     | 81  | ILE  |
| 1   | C     | 89  | ARG  |
| 1   | C     | 90  | ILE  |
| 1   | C     | 117 | ILE  |
| 1   | C     | 119 | LYS  |
| 1   | C     | 122 | LYS  |
| 1   | C     | 141 | LEU  |
| 1   | C     | 145 | VAL  |
| 1   | C     | 155 | THR  |
| 1   | C     | 160 | LYS  |
| 1   | C     | 172 | GLU  |
| 1   | C     | 180 | LYS  |
| 1   | C     | 182 | GLN  |
| 1   | C     | 196 | VAL  |
| 1   | C     | 202 | VAL  |
| 1   | C     | 206 | GLU  |
| 1   | C     | 207 | LEU  |
| 1   | D     | 4   | LEU  |
| 1   | D     | 29  | ILE  |
| 1   | D     | 50  | GLU  |
| 1   | D     | 52  | LEU  |
| 1   | D     | 67  | VAL  |
| 1   | D     | 69  | LEU  |
| 1   | D     | 73  | ARG  |
| 1   | D     | 81  | ILE  |
| 1   | D     | 89  | ARG  |
| 1   | D     | 103 | ILE  |
| 1   | D     | 117 | ILE  |
| 1   | D     | 119 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 122 | LYS  |
| 1   | D     | 129 | ILE  |
| 1   | D     | 141 | LEU  |
| 1   | D     | 145 | VAL  |
| 1   | D     | 155 | THR  |
| 1   | D     | 160 | LYS  |
| 1   | D     | 172 | GLU  |
| 1   | D     | 180 | LYS  |
| 1   | D     | 182 | GLN  |
| 1   | D     | 196 | VAL  |
| 1   | D     | 202 | VAL  |
| 1   | D     | 206 | GLU  |
| 1   | D     | 207 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 93  | ASN  |
| 1   | A     | 135 | ASN  |
| 1   | B     | 93  | ASN  |
| 1   | B     | 135 | ASN  |
| 1   | B     | 152 | HIS  |
| 1   | C     | 93  | ASN  |
| 1   | C     | 135 | ASN  |
| 1   | C     | 152 | HIS  |
| 1   | D     | 93  | ASN  |
| 1   | D     | 135 | 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

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.