



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:19 AM UTC

PDB ID : 3PCK / pdb\_00003pck  
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-  
PLEXED WITH 6-HYDROXYNICOTINIC ACID N-OXIDE  
Authors : Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.  
Deposited on : 1997-07-18  
Resolution : 2.13 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                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| 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                                                             |

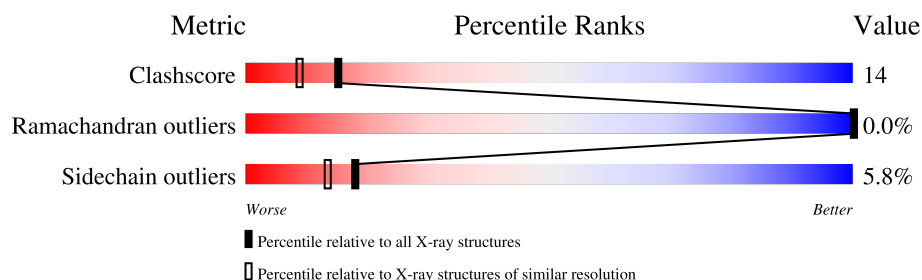
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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                      | 3812 (2.16-2.12)                                      |
| Ramachandran outliers | 187476                      | 3773 (2.16-2.12)                                      |
| Sidechain outliers    | 187428                      | 3772 (2.16-2.12)                                      |

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     | 200    | 68% 25% 6% .     |
| 1   | B     | 200    | 64% 31% . .      |
| 1   | C     | 200    | 66% 26% 5% .     |
| 1   | D     | 200    | 68% 25% 6%       |
| 1   | E     | 200    | 68% 26% 5%       |
| 1   | F     | 200    | 60% 30% 8% .     |
| 2   | M     | 238    | 64% 27% 5% . .   |
| 2   | N     | 238    | 71% 22% 5% .     |

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| Mol | Chain | Length | Quality of chain                                                                                    |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------|
| 2   | O     | 238    | <br>64% 27% 6% •  |
| 2   | P     | 238    | <br>70% 22% 5% •• |
| 2   | Q     | 238    | <br>66% 26% 6% •  |
| 2   | R     | 238    | <br>62% 29% 5% •• |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22014 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 PROTOCATECHUATE 3,4-DIOXYGENASE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 200      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1571  | 993 | 276 | 299 | 3 |         |         |       |
| 1   | B     | 200      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1571  | 993 | 276 | 299 | 3 |         |         |       |
| 1   | C     | 200      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1571  | 993 | 276 | 299 | 3 |         |         |       |
| 1   | D     | 200      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1571  | 993 | 276 | 299 | 3 |         |         |       |
| 1   | E     | 200      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1571  | 993 | 276 | 299 | 3 |         |         |       |
| 1   | F     | 200      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1571  | 993 | 276 | 299 | 3 |         |         |       |

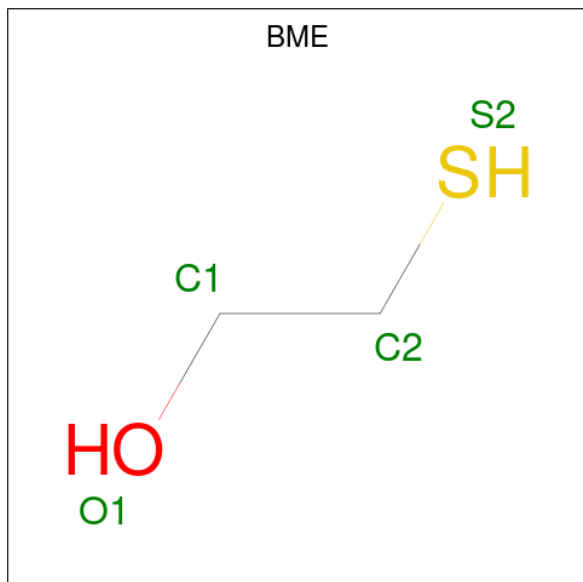
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | M     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1840  | 1171 | 334 | 328 | 7 |         |         |       |
| 2   | N     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1840  | 1171 | 334 | 328 | 7 |         |         |       |
| 2   | O     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1840  | 1171 | 334 | 328 | 7 |         |         |       |
| 2   | P     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1840  | 1171 | 334 | 328 | 7 |         |         |       |
| 2   | Q     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1840  | 1171 | 334 | 328 | 7 |         |         |       |
| 2   | R     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1840  | 1171 | 334 | 328 | 7 |         |         |       |

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

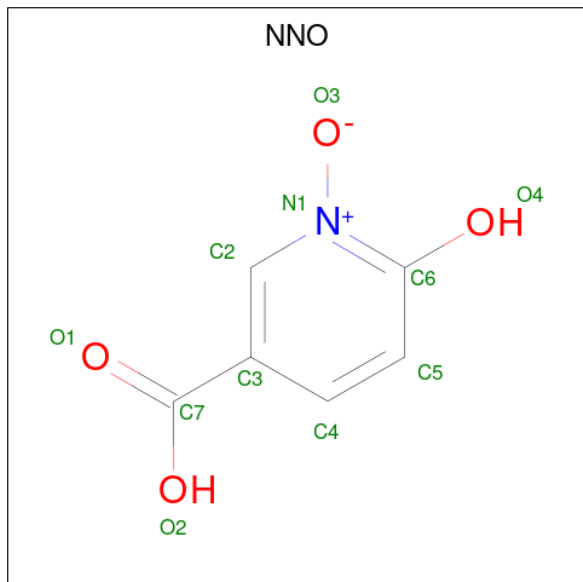
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | M     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 3   | N     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 3   | O     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 3   | P     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 3   | Q     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 3   | R     | 1        | Total Fe<br>1 1 | 0       | 0       |

- Molecule 4 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



| Mol | Chain | Residues | Atoms                  | ZeroOcc | AltConf |
|-----|-------|----------|------------------------|---------|---------|
| 4   | M     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 4   | N     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 4   | O     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 4   | P     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 4   | Q     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |
| 4   | R     | 1        | Total C O S<br>4 2 1 1 | 0       | 0       |

- Molecule 5 is 6-HYDROXYISONICOTINIC ACID N-OXIDE (CCD ID: NNO) (formula:  $C_6H_5NO_4$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 5   | M     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 11    | 6 | 1 | 4 |         |         |
| 5   | N     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 11    | 6 | 1 | 4 |         |         |
| 5   | O     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 11    | 6 | 1 | 4 |         |         |
| 5   | P     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 11    | 6 | 1 | 4 |         |         |
| 5   | Q     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 11    | 6 | 1 | 4 |         |         |
| 5   | R     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 11    | 6 | 1 | 4 |         |         |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 6   | A     | 86       | Total | O   | 0       | 0       |
|     |       |          | 86    | 86  |         |         |
| 6   | M     | 155      | Total | O   | 0       | 0       |
|     |       |          | 155   | 155 |         |         |
| 6   | B     | 85       | Total | O   | 0       | 0       |
|     |       |          | 85    | 85  |         |         |
| 6   | N     | 160      | Total | O   | 0       | 0       |
|     |       |          | 160   | 160 |         |         |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 6   | C     | 83       | Total<br>83  | O<br>83  | 0       | 0       |
| 6   | O     | 157      | Total<br>157 | O<br>157 | 0       | 0       |
| 6   | D     | 81       | Total<br>81  | O<br>81  | 0       | 0       |
| 6   | P     | 155      | Total<br>155 | O<br>155 | 0       | 0       |
| 6   | E     | 86       | Total<br>86  | O<br>86  | 0       | 0       |
| 6   | Q     | 161      | Total<br>161 | O<br>161 | 0       | 0       |
| 6   | F     | 86       | Total<br>86  | O<br>86  | 0       | 0       |
| 6   | R     | 157      | Total<br>157 | O<br>157 | 0       | 0       |

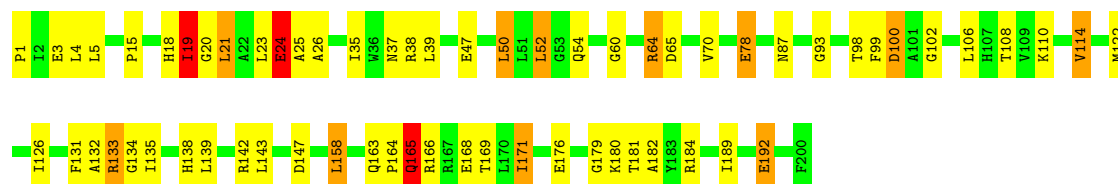
### 3 Residue-property plots

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.

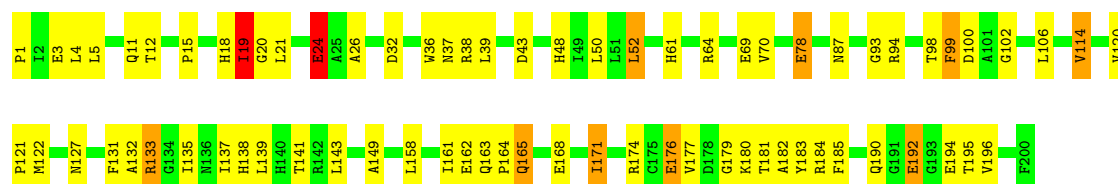
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain A: 



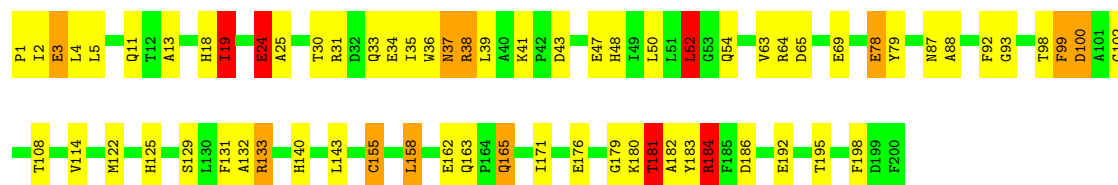
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain B: 



#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain C: 



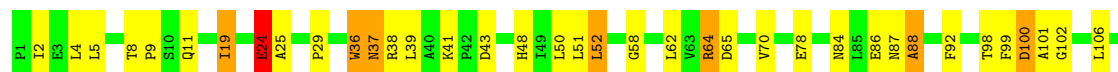
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain D: 





- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

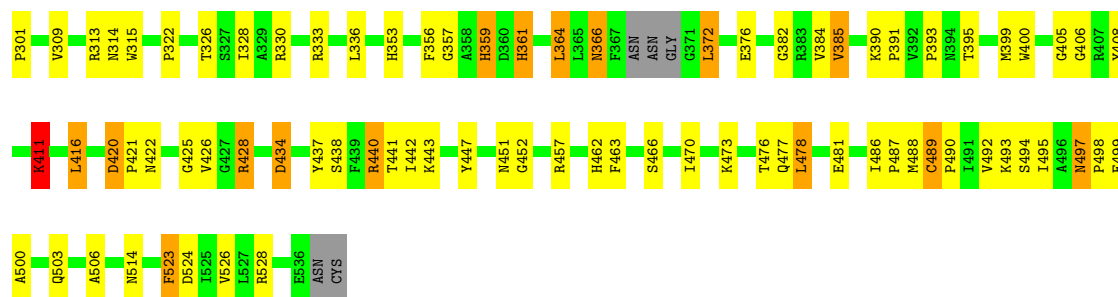


- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

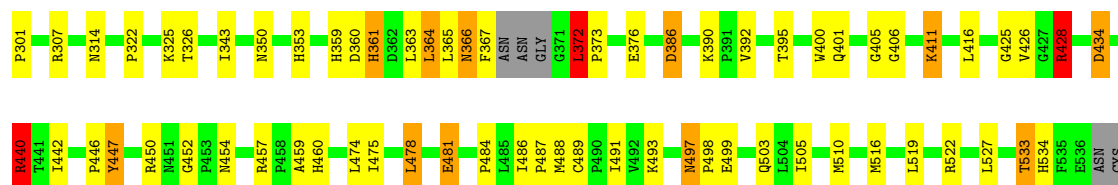


- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

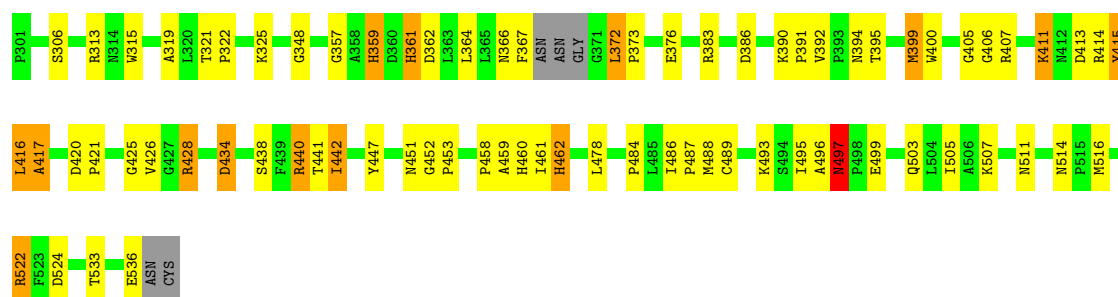




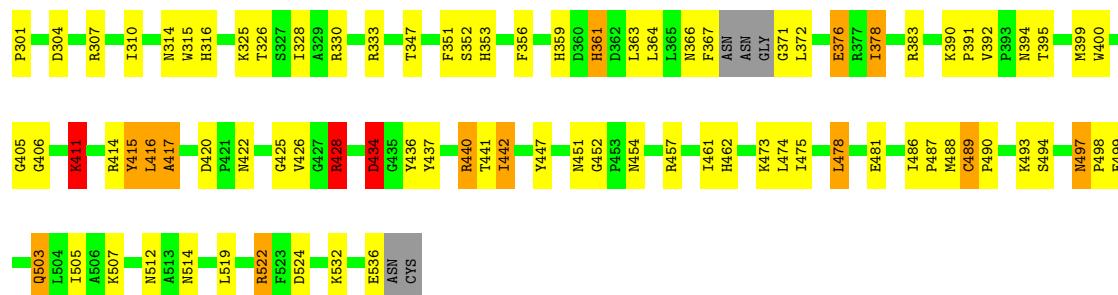
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



## 4 Data and refinement statistics

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

| Property                                                 | Value                                           | Source    |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                              | I 1 2 1                                         | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 196.90Å 127.80Å 134.40Å<br>90.00° 97.80° 90.00° | Depositor |
| Resolution (Å)                                           | 6.00 – 2.13                                     | Depositor |
| % Data completeness<br>(in resolution range)             | 88.0 (6.00-2.13)                                | Depositor |
| $R_{merge}$                                              | (Not available)                                 | Depositor |
| $R_{sym}$                                                | 0.10                                            | Depositor |
| Refinement program                                       | PROLSQ                                          | Depositor |
| R, $R_{free}$                                            | 0.173 , (Not available)                         | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 22014                                           | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 21.0                                            | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, BME, NNO

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         | 3/1611 (0.2%)   | 1.82        | 28/2195 (1.3%)   |
| 1   | B     | 1.29         | 2/1611 (0.1%)   | 1.84        | 32/2195 (1.5%)   |
| 1   | C     | 1.29         | 5/1611 (0.3%)   | 1.75        | 28/2195 (1.3%)   |
| 1   | D     | 1.30         | 2/1611 (0.1%)   | 1.79        | 23/2195 (1.0%)   |
| 1   | E     | 1.27         | 0/1611          | 1.82        | 26/2195 (1.2%)   |
| 1   | F     | 1.35         | 5/1611 (0.3%)   | 1.81        | 22/2195 (1.0%)   |
| 2   | M     | 1.41         | 8/1895 (0.4%)   | 1.87        | 35/2580 (1.4%)   |
| 2   | N     | 1.41         | 6/1895 (0.3%)   | 1.85        | 34/2580 (1.3%)   |
| 2   | O     | 1.41         | 8/1895 (0.4%)   | 1.88        | 49/2580 (1.9%)   |
| 2   | P     | 1.42         | 4/1895 (0.2%)   | 1.83        | 27/2580 (1.0%)   |
| 2   | Q     | 1.47         | 10/1895 (0.5%)  | 1.83        | 34/2580 (1.3%)   |
| 2   | R     | 1.39         | 4/1895 (0.2%)   | 1.84        | 41/2580 (1.6%)   |
| All | All   | 1.37         | 57/21036 (0.3%) | 1.83        | 379/28650 (1.3%) |

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   | C     | 0                   | 1                   |
| 2   | M     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (57) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | Q     | 451 | ASN  | CA-C  | 9.14 | 1.56        | 1.52     |
| 2   | N     | 441 | THR  | CA-CB | 8.10 | 1.64        | 1.54     |
| 2   | O     | 313 | ARG  | NE-CZ | 7.57 | 1.41        | 1.33     |
| 2   | O     | 451 | ASN  | CA-C  | 7.28 | 1.55        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | M     | 428 | ARG  | CD-NE   | -7.21 | 1.36        | 1.46     |
| 2   | M     | 447 | TYR  | CA-CB   | 6.84  | 1.64        | 1.53     |
| 1   | A     | 133 | ARG  | CD-NE   | -6.82 | 1.36        | 1.46     |
| 2   | R     | 451 | ASN  | CA-C    | 6.71  | 1.55        | 1.52     |
| 2   | Q     | 441 | THR  | CA-CB   | 6.63  | 1.63        | 1.54     |
| 1   | D     | 4   | LEU  | N-CA    | 6.57  | 1.54        | 1.45     |
| 2   | P     | 452 | GLY  | CA-C    | 6.42  | 1.60        | 1.51     |
| 1   | A     | 108 | THR  | CA-CB   | 6.26  | 1.62        | 1.53     |
| 1   | C     | 108 | THR  | CA-CB   | 6.12  | 1.61        | 1.54     |
| 2   | O     | 441 | THR  | CA-CB   | 6.11  | 1.61        | 1.54     |
| 2   | Q     | 462 | HIS  | N-CA    | 6.10  | 1.53        | 1.46     |
| 2   | N     | 523 | PHE  | N-CA    | 6.08  | 1.53        | 1.46     |
| 2   | M     | 452 | GLY  | N-CA    | 5.94  | 1.52        | 1.44     |
| 2   | N     | 428 | ARG  | CD-NE   | -5.93 | 1.38        | 1.46     |
| 1   | F     | 171 | ILE  | CA-CB   | 5.85  | 1.60        | 1.53     |
| 2   | Q     | 428 | ARG  | CD-NE   | -5.84 | 1.38        | 1.46     |
| 2   | O     | 428 | ARG  | CD-NE   | -5.83 | 1.38        | 1.46     |
| 1   | F     | 108 | THR  | CA-CB   | 5.74  | 1.61        | 1.54     |
| 1   | F     | 13  | ALA  | C-O     | 5.59  | 1.31        | 1.24     |
| 2   | Q     | 478 | LEU  | CA-C    | 5.53  | 1.59        | 1.52     |
| 2   | Q     | 321 | THR  | N-CA    | 5.49  | 1.52        | 1.46     |
| 2   | Q     | 495 | ILE  | CA-CB   | 5.48  | 1.59        | 1.53     |
| 2   | N     | 445 | GLY  | N-CA    | 5.47  | 1.52        | 1.44     |
| 2   | P     | 447 | TYR  | CA-CB   | 5.46  | 1.62        | 1.53     |
| 2   | N     | 457 | ARG  | CA-C    | 5.45  | 1.59        | 1.52     |
| 1   | F     | 2   | ILE  | CA-CB   | 5.44  | 1.60        | 1.54     |
| 1   | D     | 108 | THR  | CA-CB   | 5.40  | 1.61        | 1.54     |
| 2   | M     | 401 | GLN  | N-CA    | 5.38  | 1.52        | 1.46     |
| 2   | O     | 476 | THR  | CA-CB   | 5.32  | 1.60        | 1.53     |
| 2   | M     | 441 | THR  | C-O     | 5.32  | 1.27        | 1.24     |
| 2   | P     | 460 | HIS  | CE1-NE2 | -5.31 | 1.27        | 1.32     |
| 2   | R     | 452 | GLY  | N-CA    | 5.31  | 1.51        | 1.44     |
| 2   | P     | 325 | LYS  | C-O     | 5.31  | 1.30        | 1.24     |
| 1   | C     | 5   | LEU  | CA-C    | 5.30  | 1.58        | 1.53     |
| 1   | B     | 12  | THR  | CA-CB   | 5.30  | 1.62        | 1.53     |
| 1   | C     | 63  | VAL  | N-CA    | 5.29  | 1.52        | 1.46     |
| 2   | M     | 321 | THR  | CA-CB   | 5.29  | 1.60        | 1.53     |
| 2   | O     | 524 | ASP  | N-CA    | 5.25  | 1.52        | 1.45     |
| 2   | N     | 466 | SER  | C-O     | 5.25  | 1.30        | 1.24     |
| 2   | Q     | 417 | ALA  | N-CA    | 5.25  | 1.52        | 1.45     |
| 2   | O     | 443 | LYS  | CA-C    | 5.21  | 1.58        | 1.52     |
| 1   | A     | 5   | LEU  | CA-C    | 5.18  | 1.58        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | M     | 424 | GLY  | N-CA  | 5.18  | 1.52        | 1.45     |
| 2   | Q     | 460 | HIS  | N-CA  | 5.17  | 1.52        | 1.45     |
| 1   | B     | 5   | LEU  | CA-C  | 5.16  | 1.58        | 1.53     |
| 1   | C     | 140 | HIS  | CA-CB | 5.13  | 1.60        | 1.53     |
| 2   | R     | 514 | ASN  | N-CA  | 5.11  | 1.52        | 1.45     |
| 2   | R     | 378 | ILE  | CA-CB | 5.10  | 1.62        | 1.55     |
| 2   | O     | 452 | GLY  | CA-C  | 5.09  | 1.58        | 1.51     |
| 2   | Q     | 392 | VAL  | N-CA  | 5.09  | 1.50        | 1.46     |
| 1   | C     | 195 | THR  | CA-CB | 5.06  | 1.61        | 1.53     |
| 2   | M     | 441 | THR  | CA-CB | 5.05  | 1.60        | 1.54     |
| 1   | F     | 36  | TRP  | CA-C  | -5.02 | 1.48        | 1.53     |

All (379) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 2   | M     | 428 | ARG  | CD-NE-CZ  | 14.39  | 144.55      | 124.40   |
| 2   | O     | 428 | ARG  | CD-NE-CZ  | 13.34  | 143.07      | 124.40   |
| 1   | A     | 133 | ARG  | CD-NE-CZ  | 13.18  | 142.84      | 124.40   |
| 2   | P     | 457 | ARG  | CD-NE-CZ  | 11.39  | 140.34      | 124.40   |
| 2   | N     | 440 | ARG  | NE-CZ-NH2 | -10.98 | 109.32      | 119.20   |
| 2   | Q     | 428 | ARG  | CD-NE-CZ  | 10.86  | 139.60      | 124.40   |
| 2   | O     | 434 | ASP  | CA-CB-CG  | -10.85 | 101.75      | 112.60   |
| 2   | P     | 452 | GLY  | N-CA-C    | -10.77 | 98.86       | 112.10   |
| 2   | Q     | 434 | ASP  | CA-CB-CG  | -10.23 | 102.37      | 112.60   |
| 2   | N     | 428 | ARG  | CD-NE-CZ  | 9.98   | 138.37      | 124.40   |
| 1   | E     | 127 | ASN  | CA-CB-CG  | -9.79  | 102.81      | 112.60   |
| 2   | Q     | 452 | GLY  | N-CA-C    | -9.72  | 100.47      | 112.23   |
| 2   | R     | 451 | ASN  | O-C-N     | 9.67   | 127.99      | 120.83   |
| 2   | R     | 452 | GLY  | N-CA-C    | -9.56  | 100.67      | 112.23   |
| 2   | R     | 434 | ASP  | CA-CB-CG  | -9.45  | 103.15      | 112.60   |
| 2   | Q     | 361 | HIS  | CA-CB-CG  | -9.38  | 104.42      | 113.80   |
| 2   | N     | 452 | GLY  | N-CA-C    | -9.37  | 100.58      | 112.10   |
| 2   | R     | 361 | HIS  | CA-CB-CG  | -9.30  | 104.50      | 113.80   |
| 1   | F     | 38  | ARG  | CD-NE-CZ  | 9.02   | 137.02      | 124.40   |
| 2   | O     | 440 | ARG  | NE-CZ-NH2 | -9.00  | 111.10      | 119.20   |
| 2   | O     | 452 | GLY  | N-CA-C    | -8.84  | 101.23      | 112.10   |
| 1   | C     | 37  | ASN  | N-CA-C    | 8.81   | 123.59      | 113.02   |
| 1   | D     | 37  | ASN  | N-CA-C    | 8.77   | 122.75      | 112.93   |
| 2   | O     | 451 | ASN  | O-C-N     | 8.73   | 127.29      | 120.83   |
| 2   | P     | 440 | ARG  | NE-CZ-NH2 | -8.67  | 111.40      | 119.20   |
| 2   | M     | 434 | ASP  | CA-CB-CG  | -8.55  | 104.05      | 112.60   |
| 2   | M     | 457 | ARG  | CD-NE-CZ  | 8.52   | 136.32      | 124.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | N     | 428 | ARG  | NE-CZ-NH1 | 8.44  | 129.94      | 121.50   |
| 1   | F     | 43  | ASP  | CA-CB-CG  | -8.39 | 104.21      | 112.60   |
| 2   | N     | 434 | ASP  | CA-CB-CG  | -8.36 | 104.24      | 112.60   |
| 1   | E     | 38  | ARG  | CD-NE-CZ  | -8.34 | 112.72      | 124.40   |
| 2   | Q     | 451 | ASN  | O-C-N     | 8.20  | 126.90      | 120.83   |
| 1   | F     | 37  | ASN  | N-CA-C    | 8.15  | 122.06      | 112.93   |
| 2   | R     | 353 | HIS  | CA-CB-CG  | -8.03 | 105.77      | 113.80   |
| 2   | P     | 361 | HIS  | CA-CB-CG  | -8.00 | 105.80      | 113.80   |
| 1   | C     | 198 | PHE  | CA-CB-CG  | 7.88  | 121.68      | 113.80   |
| 1   | D     | 112 | GLY  | CA-C-N    | 7.75  | 132.36      | 121.66   |
| 1   | D     | 112 | GLY  | C-N-CA    | 7.75  | 132.36      | 121.66   |
| 1   | E     | 37  | ASN  | N-CA-C    | 7.73  | 121.59      | 112.93   |
| 1   | D     | 131 | PHE  | CA-CB-CG  | 7.65  | 121.45      | 113.80   |
| 2   | O     | 353 | HIS  | CA-CB-CG  | -7.63 | 106.17      | 113.80   |
| 1   | A     | 5   | LEU  | N-CA-C    | -7.59 | 100.19      | 109.83   |
| 2   | P     | 457 | ARG  | NE-CZ-NH1 | 7.59  | 129.09      | 121.50   |
| 2   | Q     | 440 | ARG  | NE-CZ-NH2 | -7.59 | 112.37      | 119.20   |
| 2   | R     | 522 | ARG  | CD-NE-CZ  | -7.58 | 113.79      | 124.40   |
| 1   | E     | 92  | PHE  | CA-CB-CG  | 7.56  | 121.36      | 113.80   |
| 2   | M     | 314 | ASN  | N-CA-C    | -7.53 | 104.12      | 113.38   |
| 1   | A     | 3   | GLU  | CB-CG-CD  | 7.52  | 125.39      | 112.60   |
| 1   | B     | 24  | GLU  | CB-CG-CD  | 7.52  | 125.39      | 112.60   |
| 2   | M     | 428 | ARG  | CG-CD-NE  | 7.50  | 128.49      | 112.00   |
| 1   | C     | 133 | ARG  | CD-NE-CZ  | 7.45  | 134.83      | 124.40   |
| 1   | A     | 192 | GLU  | CB-CG-CD  | 7.40  | 125.18      | 112.60   |
| 2   | N     | 392 | VAL  | O-C-N     | 7.36  | 128.03      | 120.96   |
| 2   | M     | 353 | HIS  | CA-CB-CG  | -7.35 | 106.45      | 113.80   |
| 2   | M     | 366 | ASN  | N-CA-C    | 7.32  | 122.06      | 113.20   |
| 1   | A     | 5   | LEU  | O-C-N     | 7.32  | 129.63      | 121.43   |
| 2   | P     | 491 | ILE  | N-CA-CB   | 7.28  | 119.89      | 110.57   |
| 2   | P     | 434 | ASP  | CA-CB-CG  | -7.26 | 105.34      | 112.60   |
| 1   | B     | 184 | ARG  | NE-CZ-NH2 | -7.26 | 112.67      | 119.20   |
| 1   | C     | 38  | ARG  | CD-NE-CZ  | -7.24 | 114.26      | 124.40   |
| 2   | R     | 522 | ARG  | NE-CZ-NH1 | -7.15 | 114.35      | 121.50   |
| 2   | R     | 440 | ARG  | NE-CZ-NH2 | -7.14 | 112.78      | 119.20   |
| 1   | A     | 47  | GLU  | CB-CG-CD  | 7.08  | 124.64      | 112.60   |
| 1   | C     | 47  | GLU  | CB-CG-CD  | 7.06  | 124.59      | 112.60   |
| 2   | P     | 372 | LEU  | CB-CA-C   | 7.05  | 118.49      | 108.68   |
| 2   | Q     | 415 | TYR  | CB-CA-C   | 7.01  | 121.36      | 109.72   |
| 1   | A     | 37  | ASN  | N-CA-C    | 6.95  | 120.71      | 112.93   |
| 1   | F     | 24  | GLU  | CB-CG-CD  | 6.92  | 124.37      | 112.60   |
| 1   | F     | 38  | ARG  | CA-CB-CG  | 6.84  | 127.77      | 114.10   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | N     | 312 | ASP  | CA-CB-CG  | -6.82 | 105.78      | 112.60   |
| 1   | A     | 142 | ARG  | CD-NE-CZ  | 6.81  | 133.93      | 124.40   |
| 1   | C     | 87  | ASN  | CA-CB-CG  | 6.80  | 119.40      | 112.60   |
| 2   | M     | 440 | ARG  | NE-CZ-NH2 | -6.79 | 113.09      | 119.20   |
| 2   | R     | 394 | ASN  | CA-CB-CG  | -6.78 | 105.82      | 112.60   |
| 1   | A     | 19  | ILE  | CB-CA-C   | 6.78  | 122.67      | 112.16   |
| 2   | P     | 481 | GLU  | CB-CG-CD  | 6.77  | 124.11      | 112.60   |
| 1   | D     | 23  | LEU  | CB-CA-C   | 6.76  | 122.07      | 110.84   |
| 2   | Q     | 497 | ASN  | CB-CA-C   | 6.76  | 119.12      | 109.38   |
| 2   | M     | 494 | SER  | N-CA-C    | -6.74 | 103.95      | 111.71   |
| 1   | D     | 84  | ASN  | CA-CB-CG  | 6.66  | 119.26      | 112.60   |
| 2   | M     | 394 | ASN  | CA-C-O    | -6.62 | 114.29      | 122.03   |
| 2   | R     | 457 | ARG  | CA-CB-CG  | 6.61  | 127.33      | 114.10   |
| 1   | C     | 125 | HIS  | CA-CB-CG  | -6.61 | 107.19      | 113.80   |
| 2   | P     | 353 | HIS  | CA-CB-CG  | -6.60 | 107.20      | 113.80   |
| 2   | O     | 457 | ARG  | CD-NE-CZ  | 6.60  | 133.64      | 124.40   |
| 2   | P     | 428 | ARG  | CB-CG-CD  | 6.59  | 126.46      | 111.30   |
| 2   | M     | 428 | ARG  | NE-CZ-NH1 | 6.59  | 128.09      | 121.50   |
| 2   | M     | 463 | PHE  | CA-CB-CG  | 6.58  | 120.39      | 113.80   |
| 1   | F     | 114 | VAL  | CA-C-O    | -6.57 | 114.77      | 121.67   |
| 2   | O     | 514 | ASN  | CA-CB-CG  | 6.56  | 119.16      | 112.60   |
| 2   | O     | 473 | LYS  | CB-CA-C   | 6.52  | 119.63      | 109.84   |
| 2   | M     | 481 | GLU  | CB-CG-CD  | 6.52  | 123.68      | 112.60   |
| 2   | N     | 496 | ALA  | N-CA-C    | 6.48  | 118.42      | 111.36   |
| 1   | C     | 99  | PHE  | CA-CB-CG  | 6.47  | 120.27      | 113.80   |
| 1   | B     | 185 | PHE  | CA-CB-CG  | 6.47  | 120.27      | 113.80   |
| 2   | O     | 428 | ARG  | CB-CG-CD  | 6.47  | 126.18      | 111.30   |
| 2   | O     | 314 | ASN  | CB-CA-C   | 6.45  | 121.03      | 109.29   |
| 1   | E     | 171 | ILE  | N-CA-C    | 6.45  | 117.40      | 107.99   |
| 1   | F     | 133 | ARG  | CA-CB-CG  | 6.44  | 126.98      | 114.10   |
| 2   | P     | 367 | PHE  | CA-C-O    | -6.44 | 109.86      | 120.80   |
| 1   | E     | 125 | HIS  | CA-CB-CG  | -6.43 | 107.37      | 113.80   |
| 2   | Q     | 383 | ARG  | CD-NE-CZ  | -6.39 | 115.45      | 124.40   |
| 2   | N     | 385 | VAL  | CA-C-O    | -6.39 | 114.90      | 121.67   |
| 2   | Q     | 428 | ARG  | CG-CD-NE  | 6.38  | 126.04      | 112.00   |
| 1   | F     | 99  | PHE  | CA-CB-CG  | 6.37  | 120.17      | 113.80   |
| 1   | E     | 24  | GLU  | CB-CG-CD  | 6.36  | 123.41      | 112.60   |
| 2   | M     | 514 | ASN  | O-C-N     | 6.34  | 128.35      | 121.12   |
| 2   | M     | 361 | HIS  | CA-CB-CG  | -6.33 | 107.47      | 113.80   |
| 2   | M     | 316 | HIS  | O-C-N     | 6.31  | 128.29      | 121.60   |
| 2   | N     | 428 | ARG  | CB-CG-CD  | 6.31  | 125.82      | 111.30   |
| 2   | R     | 304 | ASP  | CA-CB-CG  | -6.31 | 106.29      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 87  | ASN  | CA-CB-CG   | 6.30  | 118.90      | 112.60   |
| 2   | Q     | 522 | ARG  | NE-CZ-NH1  | -6.29 | 115.21      | 121.50   |
| 2   | R     | 411 | LYS  | CB-CA-C    | -6.29 | 100.75      | 110.81   |
| 1   | B     | 36  | TRP  | CB-CA-C    | 6.28  | 122.92      | 110.42   |
| 1   | E     | 64  | ARG  | CD-NE-CZ   | -6.27 | 115.62      | 124.40   |
| 2   | P     | 474 | LEU  | O-C-N      | 6.27  | 130.41      | 123.33   |
| 1   | D     | 28  | ASN  | O-C-N      | 6.25  | 126.67      | 121.35   |
| 2   | M     | 428 | ARG  | CB-CG-CD   | 6.25  | 125.68      | 111.30   |
| 1   | C     | 183 | TYR  | N-CA-CB    | 6.25  | 121.31      | 110.81   |
| 1   | E     | 5   | LEU  | N-CA-C     | -6.25 | 101.45      | 110.08   |
| 2   | N     | 428 | ARG  | CG-CD-NE   | 6.24  | 125.73      | 112.00   |
| 2   | R     | 314 | ASN  | N-CA-C     | -6.24 | 105.99      | 113.97   |
| 1   | A     | 184 | ARG  | CD-NE-CZ   | 6.23  | 133.13      | 124.40   |
| 1   | D     | 38  | ARG  | CD-NE-CZ   | -6.23 | 115.68      | 124.40   |
| 1   | E     | 144 | TYR  | N-CA-CB    | 6.21  | 120.36      | 111.05   |
| 2   | Q     | 514 | ASN  | O-C-N      | 6.20  | 127.02      | 121.19   |
| 2   | Q     | 325 | LYS  | N-CA-C     | 6.20  | 118.55      | 111.11   |
| 2   | Q     | 359 | HIS  | CA-CB-CG   | -6.15 | 107.65      | 113.80   |
| 1   | A     | 60  | GLY  | N-CA-C     | -6.14 | 106.68      | 115.64   |
| 1   | E     | 36  | TRP  | CB-CA-C    | 6.14  | 122.64      | 110.42   |
| 2   | M     | 339 | ILE  | O-C-N      | 6.14  | 128.10      | 121.10   |
| 1   | B     | 127 | ASN  | OD1-CG-ND2 | 6.14  | 128.74      | 122.60   |
| 2   | M     | 526 | VAL  | O-C-N      | 6.13  | 129.69      | 123.20   |
| 1   | B     | 37  | ASN  | N-CA-C     | 6.11  | 120.35      | 113.02   |
| 2   | M     | 462 | HIS  | CA-CB-CG   | -6.10 | 107.70      | 113.80   |
| 2   | O     | 385 | VAL  | O-C-N      | 6.10  | 129.71      | 123.00   |
| 2   | Q     | 319 | ALA  | O-C-N      | 6.09  | 128.67      | 122.09   |
| 2   | O     | 384 | VAL  | O-C-N      | 6.09  | 130.22      | 123.10   |
| 2   | Q     | 313 | ARG  | CD-NE-CZ   | 6.08  | 132.92      | 124.40   |
| 2   | Q     | 428 | ARG  | NE-CZ-NH2  | -6.08 | 113.73      | 119.20   |
| 1   | C     | 155 | CYS  | O-C-N      | 6.08  | 126.83      | 121.18   |
| 2   | N     | 325 | LYS  | N-CA-C     | 6.06  | 121.30      | 111.37   |
| 1   | F     | 38  | ARG  | NE-CZ-NH1  | 6.05  | 127.55      | 121.50   |
| 1   | B     | 176 | GLU  | CB-CG-CD   | 6.03  | 122.86      | 112.60   |
| 2   | N     | 361 | HIS  | CA-CB-CG   | -5.99 | 107.81      | 113.80   |
| 1   | B     | 18  | HIS  | CA-CB-CG   | -5.99 | 107.81      | 113.80   |
| 2   | P     | 392 | VAL  | O-C-N      | 5.99  | 127.92      | 121.10   |
| 1   | C     | 5   | LEU  | N-CA-C     | -5.97 | 102.24      | 109.83   |
| 1   | E     | 127 | ASN  | OD1-CG-ND2 | 5.97  | 128.57      | 122.60   |
| 1   | A     | 171 | ILE  | N-CA-C     | 5.96  | 116.69      | 107.99   |
| 1   | A     | 64  | ARG  | CD-NE-CZ   | -5.96 | 116.06      | 124.40   |
| 2   | O     | 440 | ARG  | NH1-CZ-NH2 | 5.95  | 127.03      | 119.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | N     | 367 | PHE  | CA-C-O     | -5.95 | 110.69      | 120.80   |
| 2   | Q     | 428 | ARG  | NE-CZ-NH1  | 5.95  | 127.45      | 121.50   |
| 2   | O     | 309 | VAL  | CA-C-N     | 5.94  | 129.36      | 120.69   |
| 2   | O     | 309 | VAL  | C-N-CA     | 5.94  | 129.36      | 120.69   |
| 2   | Q     | 348 | GLY  | O-C-N      | 5.94  | 127.71      | 121.77   |
| 1   | B     | 43  | ASP  | CA-CB-CG   | -5.93 | 106.67      | 112.60   |
| 2   | O     | 428 | ARG  | NE-CZ-NH1  | 5.93  | 127.43      | 121.50   |
| 1   | A     | 166 | ARG  | NE-CZ-NH2  | -5.92 | 113.87      | 119.20   |
| 1   | F     | 5   | LEU  | N-CA-C     | -5.91 | 101.92      | 110.08   |
| 2   | R     | 451 | ASN  | CA-C-O     | -5.90 | 116.41      | 119.77   |
| 2   | O     | 523 | PHE  | CA-CB-CG   | 5.90  | 119.70      | 113.80   |
| 2   | P     | 533 | THR  | CA-CB-OG1  | -5.88 | 100.78      | 109.60   |
| 1   | E     | 52  | LEU  | CB-CA-C    | 5.87  | 123.07      | 110.45   |
| 1   | C     | 184 | ARG  | CD-NE-CZ   | -5.86 | 116.20      | 124.40   |
| 2   | O     | 428 | ARG  | CG-CD-NE   | 5.85  | 124.87      | 112.00   |
| 1   | B     | 32  | ASP  | CA-CB-CG   | 5.84  | 118.44      | 112.60   |
| 2   | P     | 325 | LYS  | N-CA-C     | 5.83  | 121.00      | 111.37   |
| 1   | E     | 78  | GLU  | CA-CB-CG   | 5.83  | 125.76      | 114.10   |
| 1   | B     | 133 | ARG  | NE-CZ-NH2  | -5.83 | 113.95      | 119.20   |
| 2   | O     | 385 | VAL  | CA-C-O     | -5.83 | 115.72      | 121.67   |
| 2   | R     | 522 | ARG  | NE-CZ-NH2  | 5.82  | 124.43      | 119.20   |
| 1   | A     | 166 | ARG  | NE-CZ-NH1  | 5.81  | 127.31      | 121.50   |
| 2   | N     | 333 | ARG  | N-CA-C     | -5.81 | 106.54      | 113.97   |
| 2   | O     | 514 | ASN  | OD1-CG-ND2 | -5.80 | 116.80      | 122.60   |
| 2   | N     | 533 | THR  | CA-CB-OG1  | -5.80 | 100.90      | 109.60   |
| 2   | R     | 376 | GLU  | CG-CD-OE2  | -5.80 | 105.07      | 118.40   |
| 1   | B     | 5   | LEU  | N-CA-C     | -5.79 | 102.47      | 109.83   |
| 1   | A     | 52  | LEU  | CB-CA-C    | 5.79  | 122.90      | 110.45   |
| 2   | Q     | 322 | PRO  | CB-CA-C    | 5.78  | 121.92      | 112.26   |
| 2   | Q     | 357 | GLY  | N-CA-C     | -5.78 | 105.14      | 112.54   |
| 2   | M     | 326 | THR  | CA-CB-OG1  | -5.75 | 100.98      | 109.60   |
| 1   | D     | 47  | GLU  | CB-CG-CD   | 5.75  | 122.37      | 112.60   |
| 1   | C     | 171 | ILE  | N-CA-C     | 5.73  | 116.36      | 107.99   |
| 1   | A     | 24  | GLU  | CB-CG-CD   | 5.72  | 122.33      | 112.60   |
| 1   | E     | 43  | ASP  | CA-CB-CG   | -5.71 | 106.89      | 112.60   |
| 2   | Q     | 391 | PRO  | O-C-N      | 5.71  | 130.08      | 123.06   |
| 1   | B     | 174 | ARG  | CD-NE-CZ   | -5.70 | 116.42      | 124.40   |
| 2   | O     | 463 | PHE  | CA-CB-CG   | 5.70  | 119.50      | 113.80   |
| 2   | O     | 506 | ALA  | N-CA-CB    | 5.70  | 118.66      | 110.06   |
| 2   | Q     | 533 | THR  | CA-CB-OG1  | -5.70 | 101.06      | 109.60   |
| 2   | P     | 386 | ASP  | CA-CB-CG   | 5.69  | 118.29      | 112.60   |
| 1   | D     | 133 | ARG  | N-CA-CB    | -5.69 | 101.24      | 109.83   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | N     | 428 | ARG  | NE-CZ-NH2  | -5.68 | 114.08      | 119.20   |
| 1   | F     | 38  | ARG  | NE-CZ-NH2  | -5.68 | 114.09      | 119.20   |
| 2   | Q     | 386 | ASP  | CB-CA-C    | 5.67  | 120.45      | 110.36   |
| 2   | Q     | 505 | ILE  | N-CA-C     | 5.67  | 115.95      | 107.51   |
| 1   | B     | 137 | ILE  | O-C-N      | 5.66  | 129.16      | 123.10   |
| 1   | C     | 133 | ARG  | CA-CB-CG   | 5.66  | 125.41      | 114.10   |
| 2   | O     | 333 | ARG  | NE-CZ-NH2  | -5.65 | 114.12      | 119.20   |
| 2   | M     | 457 | ARG  | CG-CD-NE   | 5.64  | 124.41      | 112.00   |
| 1   | A     | 78  | GLU  | CA-CB-CG   | 5.64  | 125.38      | 114.10   |
| 1   | D     | 5   | LEU  | N-CA-C     | -5.64 | 102.67      | 109.83   |
| 1   | F     | 79  | TYR  | CA-C-O     | 5.63  | 126.74      | 120.43   |
| 1   | C     | 69  | GLU  | CB-CG-CD   | 5.63  | 122.17      | 112.60   |
| 2   | M     | 314 | ASN  | CB-CA-C    | 5.63  | 119.44      | 109.65   |
| 2   | Q     | 461 | ILE  | N-CA-CB    | 5.63  | 119.18      | 111.41   |
| 2   | P     | 459 | ALA  | N-CA-C     | -5.62 | 101.98      | 110.24   |
| 1   | B     | 161 | ILE  | CA-C-N     | 5.62  | 128.12      | 120.54   |
| 1   | B     | 161 | ILE  | C-N-CA     | 5.62  | 128.12      | 120.54   |
| 1   | D     | 171 | ILE  | N-CA-C     | 5.62  | 116.19      | 107.99   |
| 2   | P     | 366 | ASN  | N-CA-C     | 5.62  | 119.75      | 113.01   |
| 1   | E     | 181 | THR  | N-CA-CB    | 5.61  | 118.36      | 109.71   |
| 1   | A     | 165 | GLN  | OE1-CD-NE2 | -5.61 | 116.99      | 122.60   |
| 2   | M     | 350 | ASN  | N-CA-CB    | 5.61  | 119.39      | 110.65   |
| 1   | D     | 75  | ALA  | CB-CA-C    | 5.60  | 121.00      | 110.63   |
| 1   | F     | 23  | LEU  | CB-CA-C    | 5.60  | 120.04      | 110.74   |
| 2   | R     | 352 | SER  | O-C-N      | 5.60  | 128.05      | 122.12   |
| 1   | B     | 149 | ALA  | CA-C-O     | -5.58 | 114.92      | 120.90   |
| 1   | B     | 184 | ARG  | NE-CZ-NH1  | 5.57  | 127.07      | 121.50   |
| 2   | O     | 492 | VAL  | N-CA-C     | -5.57 | 105.08      | 110.42   |
| 1   | B     | 171 | ILE  | N-CA-C     | 5.56  | 116.10      | 107.99   |
| 2   | O     | 359 | HIS  | CA-CB-CG   | -5.55 | 108.25      | 113.80   |
| 2   | O     | 494 | SER  | N-CA-C     | -5.54 | 105.78      | 112.54   |
| 2   | M     | 413 | ASP  | CA-C-O     | 5.54  | 126.50      | 120.58   |
| 2   | R     | 428 | ARG  | CB-CG-CD   | 5.54  | 124.03      | 111.30   |
| 2   | P     | 314 | ASN  | CB-CA-C    | 5.53  | 118.92      | 109.24   |
| 1   | F     | 90  | ASN  | CA-CB-CG   | 5.53  | 118.12      | 112.60   |
| 1   | B     | 177 | VAL  | CB-CA-C    | 5.52  | 116.71      | 110.41   |
| 2   | O     | 384 | VAL  | CA-C-O     | -5.51 | 114.63      | 120.53   |
| 2   | M     | 452 | GLY  | N-CA-C     | -5.50 | 101.12      | 112.34   |
| 1   | B     | 139 | LEU  | O-C-N      | 5.49  | 129.77      | 123.29   |
| 2   | N     | 503 | GLN  | CB-CG-CD   | 5.48  | 121.92      | 112.60   |
| 2   | O     | 322 | PRO  | CB-CA-C    | 5.48  | 120.61      | 111.56   |
| 2   | O     | 420 | ASP  | CB-CA-C    | 5.48  | 116.25      | 110.17   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | R     | 392 | VAL  | O-C-N      | 5.48  | 126.22      | 120.96   |
| 1   | B     | 194 | GLU  | CA-CB-CG   | 5.47  | 125.05      | 114.10   |
| 2   | R     | 376 | GLU  | O-C-N      | 5.47  | 129.86      | 122.96   |
| 1   | B     | 87  | ASN  | CA-CB-CG   | 5.47  | 118.07      | 112.60   |
| 1   | C     | 19  | ILE  | CA-CB-CG1  | 5.47  | 119.70      | 110.40   |
| 2   | O     | 422 | ASN  | OD1-CG-ND2 | 5.47  | 128.07      | 122.60   |
| 2   | P     | 440 | ARG  | NE-CZ-NH1  | 5.47  | 126.97      | 121.50   |
| 2   | N     | 327 | SER  | CA-C-O     | -5.47 | 113.68      | 119.97   |
| 1   | C     | 19  | ILE  | CB-CA-C    | 5.46  | 120.63      | 112.16   |
| 2   | M     | 323 | ASP  | O-C-N      | 5.46  | 128.99      | 122.27   |
| 2   | M     | 357 | GLY  | CA-C-N     | 5.46  | 128.15      | 120.28   |
| 2   | M     | 357 | GLY  | C-N-CA     | 5.46  | 128.15      | 120.28   |
| 2   | O     | 372 | LEU  | CB-CA-C    | 5.45  | 116.55      | 108.87   |
| 1   | F     | 138 | HIS  | CA-CB-CG   | -5.45 | 108.35      | 113.80   |
| 2   | R     | 481 | GLU  | CB-CG-CD   | 5.44  | 121.85      | 112.60   |
| 2   | O     | 497 | ASN  | CB-CA-C    | 5.44  | 116.05      | 109.85   |
| 1   | E     | 88  | ALA  | N-CA-C     | -5.44 | 106.48      | 113.23   |
| 2   | R     | 417 | ALA  | N-CA-C     | -5.43 | 102.94      | 109.83   |
| 1   | B     | 183 | TYR  | N-CA-CB    | 5.42  | 120.84      | 111.13   |
| 2   | Q     | 522 | ARG  | CD-NE-CZ   | -5.41 | 116.82      | 124.40   |
| 1   | C     | 3   | GLU  | CA-C-O     | -5.41 | 114.48      | 120.38   |
| 2   | P     | 314 | ASN  | N-CA-C     | -5.40 | 106.82      | 113.41   |
| 1   | A     | 23  | LEU  | CB-CA-C    | 5.39  | 119.79      | 110.84   |
| 1   | D     | 19  | ILE  | CB-CA-C    | 5.39  | 119.41      | 112.14   |
| 1   | E     | 152 | ASN  | O-C-N      | 5.38  | 128.52      | 122.22   |
| 2   | R     | 461 | ILE  | O-C-N      | 5.38  | 129.01      | 123.20   |
| 1   | B     | 99  | PHE  | CA-CB-CG   | 5.38  | 119.18      | 113.80   |
| 1   | E     | 48  | HIS  | CA-CB-CG   | -5.37 | 108.43      | 113.80   |
| 1   | C     | 48  | HIS  | CA-CB-CG   | -5.37 | 108.44      | 113.80   |
| 1   | D     | 198 | PHE  | CA-CB-CG   | 5.37  | 119.17      | 113.80   |
| 2   | Q     | 459 | ALA  | N-CA-C     | -5.36 | 102.11      | 110.10   |
| 2   | R     | 420 | ASP  | CB-CA-C    | 5.36  | 116.31      | 110.15   |
| 2   | P     | 401 | GLN  | O-C-N      | 5.35  | 128.64      | 123.29   |
| 1   | A     | 169 | THR  | CA-CB-CG2  | 5.35  | 119.59      | 110.50   |
| 2   | R     | 333 | ARG  | N-CA-C     | -5.35 | 107.12      | 113.97   |
| 1   | B     | 11  | GLN  | N-CA-CB    | 5.35  | 120.99      | 111.69   |
| 2   | N     | 327 | SER  | O-C-N      | 5.34  | 128.84      | 122.27   |
| 2   | P     | 505 | ILE  | N-CA-C     | 5.33  | 116.39      | 108.23   |
| 1   | B     | 48  | HIS  | CA-CB-CG   | -5.33 | 108.47      | 113.80   |
| 1   | C     | 24  | GLU  | CB-CG-CD   | 5.33  | 121.66      | 112.60   |
| 1   | C     | 33  | GLN  | OE1-CD-NE2 | -5.33 | 117.27      | 122.60   |
| 2   | N     | 328 | ILE  | O-C-N      | 5.33  | 127.13      | 121.91   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 52  | LEU  | CB-CA-C    | 5.32  | 121.28      | 109.94   |
| 1   | B     | 192 | GLU  | CB-CG-CD   | 5.32  | 121.65      | 112.60   |
| 1   | D     | 177 | VAL  | CB-CA-C    | 5.32  | 117.60      | 110.42   |
| 1   | A     | 139 | LEU  | CB-CA-C    | 5.31  | 118.51      | 109.80   |
| 2   | Q     | 458 | PRO  | N-CA-C     | -5.30 | 103.12      | 111.34   |
| 1   | E     | 2   | ILE  | N-CA-CB    | -5.29 | 104.76      | 110.53   |
| 2   | M     | 477 | GLN  | OE1-CD-NE2 | -5.29 | 117.31      | 122.60   |
| 2   | N     | 333 | ARG  | CB-CA-C    | 5.29  | 117.95      | 109.07   |
| 1   | C     | 5   | LEU  | O-C-N      | 5.28  | 127.34      | 121.43   |
| 1   | D     | 133 | ARG  | NE-CZ-NH2  | -5.27 | 114.46      | 119.20   |
| 2   | O     | 333 | ARG  | N-CA-C     | -5.27 | 106.98      | 113.41   |
| 1   | D     | 43  | ASP  | CA-CB-CG   | -5.26 | 107.33      | 112.60   |
| 2   | R     | 441 | THR  | O-C-N      | 5.26  | 128.76      | 122.72   |
| 1   | D     | 41  | LYS  | N-CA-C     | -5.25 | 103.04      | 110.29   |
| 1   | A     | 189 | ILE  | O-C-N      | 5.25  | 127.24      | 121.83   |
| 1   | E     | 39  | LEU  | O-C-N      | 5.25  | 128.13      | 122.15   |
| 1   | B     | 38  | ARG  | NE-CZ-NH2  | -5.25 | 114.48      | 119.20   |
| 2   | N     | 357 | GLY  | CA-C-N     | 5.24  | 127.31      | 120.28   |
| 2   | N     | 357 | GLY  | C-N-CA     | 5.24  | 127.31      | 120.28   |
| 2   | R     | 512 | ASN  | CA-CB-CG   | -5.22 | 107.38      | 112.60   |
| 1   | E     | 189 | ILE  | O-C-N      | 5.21  | 126.93      | 121.87   |
| 2   | N     | 477 | GLN  | O-C-N      | 5.21  | 129.64      | 123.33   |
| 2   | R     | 328 | ILE  | N-CA-C     | 5.21  | 115.65      | 110.23   |
| 2   | P     | 365 | LEU  | N-CA-C     | 5.21  | 120.29      | 113.88   |
| 1   | F     | 171 | ILE  | N-CA-C     | 5.21  | 115.85      | 107.73   |
| 2   | N     | 437 | TYR  | O-C-N      | 5.20  | 129.90      | 123.15   |
| 2   | P     | 454 | ASN  | CA-CB-CG   | 5.20  | 117.80      | 112.60   |
| 2   | R     | 428 | ARG  | CG-CD-NE   | 5.20  | 123.43      | 112.00   |
| 2   | R     | 451 | ASN  | N-CA-C     | -5.20 | 100.19      | 108.30   |
| 2   | R     | 454 | ASN  | CA-C-O     | -5.19 | 115.51      | 122.31   |
| 2   | O     | 466 | SER  | N-CA-C     | 5.19  | 116.79      | 111.03   |
| 1   | E     | 177 | VAL  | CB-CA-C    | 5.19  | 116.90      | 110.73   |
| 1   | F     | 174 | ARG  | CD-NE-CZ   | -5.19 | 117.14      | 124.40   |
| 1   | D     | 139 | LEU  | CB-CA-C    | 5.18  | 118.30      | 109.75   |
| 1   | D     | 140 | HIS  | CA-CB-CG   | 5.18  | 118.98      | 113.80   |
| 2   | R     | 457 | ARG  | N-CA-C     | -5.18 | 103.25      | 109.83   |
| 2   | M     | 420 | ASP  | O-C-N      | 5.18  | 127.71      | 121.29   |
| 2   | O     | 336 | LEU  | CA-C-O     | -5.17 | 116.06      | 121.55   |
| 2   | O     | 443 | LYS  | O-C-N      | 5.17  | 126.45      | 121.28   |
| 2   | R     | 325 | LYS  | N-CA-C     | 5.17  | 119.90      | 111.37   |
| 2   | O     | 428 | ARG  | NE-CZ-NH2  | -5.17 | 114.55      | 119.20   |
| 2   | O     | 440 | ARG  | CB-CG-CD   | -5.17 | 99.42       | 111.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | N     | 309 | VAL  | O-C-N     | 5.16  | 127.94      | 122.67   |
| 1   | A     | 166 | ARG  | CD-NE-CZ  | 5.16  | 131.62      | 124.40   |
| 2   | O     | 357 | GLY  | N-CA-C    | -5.16 | 105.93      | 112.54   |
| 2   | Q     | 497 | ASN  | CA-CB-CG  | 5.16  | 117.76      | 112.60   |
| 1   | A     | 133 | ARG  | NE-CZ-NH2 | -5.16 | 114.56      | 119.20   |
| 1   | B     | 19  | ILE  | CB-CA-C   | 5.16  | 120.15      | 112.16   |
| 1   | C     | 181 | THR  | N-CA-CB   | 5.16  | 117.65      | 109.71   |
| 2   | R     | 494 | SER  | N-CA-C    | -5.16 | 106.25      | 112.54   |
| 2   | Q     | 367 | PHE  | CA-C-O    | -5.14 | 112.05      | 120.80   |
| 2   | O     | 366 | ASN  | N-CA-C    | 5.14  | 119.40      | 113.18   |
| 1   | F     | 106 | LEU  | O-C-N     | 5.13  | 129.54      | 123.33   |
| 1   | C     | 13  | ALA  | N-CA-C    | -5.13 | 105.87      | 111.82   |
| 2   | O     | 451 | ASN  | CA-C-O    | -5.13 | 116.85      | 119.77   |
| 2   | N     | 431 | THR  | N-CA-CB   | 5.12  | 117.54      | 110.17   |
| 2   | Q     | 411 | LYS  | CB-CA-C   | -5.11 | 102.35      | 110.84   |
| 2   | O     | 528 | ARG  | O-C-N     | 5.11  | 129.21      | 122.97   |
| 1   | C     | 186 | ASP  | CA-CB-CG  | 5.11  | 117.71      | 112.60   |
| 1   | E     | 11  | GLN  | CA-C-O    | -5.11 | 115.27      | 120.99   |
| 1   | E     | 99  | PHE  | CA-CB-CG  | 5.11  | 118.91      | 113.80   |
| 2   | R     | 415 | TYR  | CB-CA-C   | 5.11  | 118.38      | 109.65   |
| 2   | O     | 489 | CYS  | N-CA-C    | 5.10  | 116.33      | 109.24   |
| 1   | F     | 52  | LEU  | CB-CA-C   | 5.10  | 121.42      | 110.45   |
| 2   | R     | 316 | HIS  | O-C-N     | 5.10  | 127.00      | 121.60   |
| 1   | C     | 52  | LEU  | CB-CA-C   | 5.09  | 121.39      | 110.45   |
| 1   | C     | 43  | ASP  | CA-CB-CG  | -5.08 | 107.52      | 112.60   |
| 1   | F     | 30  | THR  | CA-CB-OG1 | -5.08 | 101.98      | 109.60   |
| 2   | R     | 532 | LYS  | O-C-N     | 5.08  | 128.63      | 122.94   |
| 2   | R     | 489 | CYS  | CA-C-N    | 5.08  | 124.57      | 119.19   |
| 2   | R     | 489 | CYS  | C-N-CA    | 5.08  | 124.57      | 119.19   |
| 2   | O     | 489 | CYS  | CA-C-N    | 5.07  | 124.86      | 119.28   |
| 2   | O     | 489 | CYS  | C-N-CA    | 5.07  | 124.86      | 119.28   |
| 1   | F     | 121 | PRO  | CB-CA-C   | -5.07 | 104.47      | 111.21   |
| 2   | R     | 367 | PHE  | CA-C-O    | -5.07 | 112.18      | 120.80   |
| 1   | B     | 114 | VAL  | O-C-N     | 5.07  | 128.42      | 123.00   |
| 2   | N     | 475 | ILE  | N-CA-CB   | 5.07  | 118.92      | 111.52   |
| 2   | N     | 390 | LYS  | CA-C-O    | 5.06  | 124.26      | 119.76   |
| 2   | R     | 347 | THR  | CA-CB-CG2 | 5.05  | 119.09      | 110.50   |
| 1   | C     | 129 | SER  | N-CA-CB   | 5.05  | 119.16      | 110.68   |
| 2   | Q     | 496 | ALA  | N-CA-C    | 5.04  | 116.86      | 111.36   |
| 1   | D     | 171 | ILE  | CB-CA-C   | 5.04  | 117.89      | 110.98   |
| 1   | A     | 126 | ILE  | O-C-N     | 5.04  | 128.70      | 123.26   |
| 2   | O     | 411 | LYS  | CB-CA-C   | -5.04 | 102.75      | 110.81   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | M     | 452 | GLY  | CA-C-N    | 5.04  | 124.70      | 119.56   |
| 2   | M     | 452 | GLY  | C-N-CA    | 5.04  | 124.70      | 119.56   |
| 1   | A     | 21  | LEU  | N-CA-C    | 5.03  | 121.16      | 113.61   |
| 2   | M     | 333 | ARG  | NE-CZ-NH2 | -5.03 | 114.67      | 119.20   |
| 2   | P     | 322 | PRO  | CB-CA-C   | 5.03  | 119.86      | 111.56   |
| 2   | N     | 535 | PHE  | CA-C-O    | -5.03 | 114.80      | 121.08   |
| 2   | O     | 361 | HIS  | CA-CB-CG  | -5.03 | 108.77      | 113.80   |
| 2   | O     | 372 | LEU  | N-CA-CB   | -5.03 | 103.50      | 110.29   |
| 2   | N     | 457 | ARG  | O-C-N     | 5.02  | 126.75      | 121.42   |
| 1   | D     | 180 | LYS  | N-CA-CB   | 5.02  | 118.78      | 110.69   |
| 2   | N     | 440 | ARG  | CB-CG-CD  | -5.01 | 99.77       | 111.30   |
| 2   | M     | 357 | GLY  | N-CA-C    | -5.01 | 105.91      | 112.82   |
| 1   | E     | 37  | ASN  | CA-CB-CG  | -5.01 | 107.59      | 112.60   |
| 2   | Q     | 511 | ASN  | CA-CB-CG  | 5.01  | 117.61      | 112.60   |
| 2   | N     | 423 | PHE  | N-CA-C    | 5.01  | 116.56      | 108.34   |
| 1   | F     | 112 | GLY  | N-CA-C    | -5.01 | 104.97      | 112.89   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | C     | 184 | ARG  | Sidechain |
| 2   | M     | 528 | ARG  | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1571  | 0        | 1499     | 48      | 0            |
| 1   | B     | 1571  | 0        | 1499     | 45      | 0            |
| 1   | C     | 1571  | 0        | 1499     | 51      | 0            |
| 1   | D     | 1571  | 0        | 1499     | 40      | 0            |
| 1   | E     | 1571  | 0        | 1499     | 41      | 0            |
| 1   | F     | 1571  | 0        | 1499     | 63      | 0            |
| 2   | M     | 1840  | 0        | 1793     | 64      | 0            |
| 2   | N     | 1840  | 0        | 1793     | 35      | 0            |
| 2   | O     | 1840  | 0        | 1793     | 53      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | P     | 1840  | 0        | 1793     | 51      | 0            |
| 2   | Q     | 1840  | 0        | 1793     | 48      | 0            |
| 2   | R     | 1840  | 0        | 1793     | 63      | 0            |
| 3   | M     | 1     | 0        | 0        | 0       | 0            |
| 3   | N     | 1     | 0        | 0        | 0       | 0            |
| 3   | O     | 1     | 0        | 0        | 0       | 0            |
| 3   | P     | 1     | 0        | 0        | 0       | 0            |
| 3   | Q     | 1     | 0        | 0        | 0       | 0            |
| 3   | R     | 1     | 0        | 0        | 0       | 0            |
| 4   | M     | 4     | 0        | 5        | 0       | 0            |
| 4   | N     | 4     | 0        | 5        | 2       | 0            |
| 4   | O     | 4     | 0        | 5        | 2       | 0            |
| 4   | P     | 4     | 0        | 5        | 0       | 0            |
| 4   | Q     | 4     | 0        | 5        | 2       | 0            |
| 4   | R     | 4     | 0        | 5        | 0       | 0            |
| 5   | M     | 11    | 0        | 3        | 0       | 0            |
| 5   | N     | 11    | 0        | 3        | 0       | 0            |
| 5   | O     | 11    | 0        | 3        | 0       | 0            |
| 5   | P     | 11    | 0        | 3        | 0       | 0            |
| 5   | Q     | 11    | 0        | 3        | 0       | 0            |
| 5   | R     | 11    | 0        | 3        | 0       | 0            |
| 6   | A     | 86    | 0        | 0        | 1       | 0            |
| 6   | B     | 85    | 0        | 0        | 1       | 0            |
| 6   | C     | 83    | 0        | 0        | 1       | 0            |
| 6   | D     | 81    | 0        | 0        | 1       | 0            |
| 6   | E     | 86    | 0        | 0        | 2       | 0            |
| 6   | F     | 86    | 0        | 0        | 1       | 0            |
| 6   | M     | 155   | 0        | 0        | 4       | 0            |
| 6   | N     | 160   | 0        | 0        | 3       | 0            |
| 6   | O     | 157   | 0        | 0        | 4       | 0            |
| 6   | P     | 155   | 0        | 0        | 7       | 0            |
| 6   | Q     | 161   | 0        | 0        | 5       | 0            |
| 6   | R     | 157   | 0        | 0        | 4       | 0            |
| All | All   | 22014 | 0        | 19800    | 548     | 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 14.

All (548) 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:E:165:GLN:H    | 1:E:165:GLN:NE2  | 1.44                     | 1.14              |
| 1:C:64:ARG:NH1   | 1:C:100:ASP:O    | 1.82                     | 1.13              |
| 1:E:165:GLN:HE21 | 1:E:165:GLN:N    | 1.50                     | 1.09              |
| 1:B:165:GLN:H    | 1:B:165:GLN:NE2  | 1.50                     | 1.07              |
| 1:D:64:ARG:NH1   | 1:D:100:ASP:O    | 1.94                     | 1.01              |
| 2:P:364:LEU:HD22 | 2:P:440:ARG:HD3  | 1.39                     | 0.98              |
| 1:F:168:GLU:HA   | 1:F:171:ILE:HD13 | 1.45                     | 0.97              |
| 1:C:163:GLN:HB3  | 1:C:165:GLN:NE2  | 1.82                     | 0.95              |
| 1:F:64:ARG:NH1   | 1:F:100:ASP:O    | 1.98                     | 0.94              |
| 1:E:64:ARG:NH1   | 1:E:100:ASP:O    | 1.99                     | 0.94              |
| 1:F:168:GLU:HA   | 1:F:171:ILE:CD1  | 1.96                     | 0.94              |
| 2:M:497:ASN:ND2  | 2:M:499:GLU:H    | 1.66                     | 0.93              |
| 2:R:497:ASN:ND2  | 2:R:499:GLU:H    | 1.65                     | 0.92              |
| 1:F:165:GLN:H    | 1:F:165:GLN:NE2  | 1.66                     | 0.92              |
| 2:M:364:LEU:HD22 | 2:M:440:ARG:HD3  | 1.53                     | 0.91              |
| 1:A:64:ARG:NH1   | 1:A:100:ASP:O    | 2.03                     | 0.90              |
| 2:N:390:LYS:HE2  | 6:N:824:HOH:O    | 1.73                     | 0.88              |
| 1:B:176:GLU:HG3  | 1:B:180:LYS:O    | 1.73                     | 0.88              |
| 2:Q:361:HIS:CD2  | 2:Q:361:HIS:H    | 1.93                     | 0.87              |
| 2:R:497:ASN:HD22 | 2:R:499:GLU:H    | 1.21                     | 0.87              |
| 1:F:176:GLU:HG3  | 1:F:180:LYS:O    | 1.76                     | 0.86              |
| 1:E:168:GLU:HA   | 1:E:171:ILE:HD12 | 1.59                     | 0.85              |
| 2:R:361:HIS:H    | 2:R:361:HIS:CD2  | 1.94                     | 0.85              |
| 1:A:134:GLY:HA3  | 2:M:326:THR:HG22 | 1.59                     | 0.85              |
| 1:A:163:GLN:HB3  | 1:A:165:GLN:NE2  | 1.91                     | 0.85              |
| 1:F:165:GLN:H    | 1:F:165:GLN:HE21 | 1.23                     | 0.85              |
| 2:N:390:LYS:HD3  | 6:N:746:HOH:O    | 1.77                     | 0.84              |
| 1:B:163:GLN:HB3  | 1:B:165:GLN:HE22 | 1.43                     | 0.82              |
| 2:R:390:LYS:HE2  | 6:R:861:HOH:O    | 1.80                     | 0.82              |
| 1:A:19:ILE:HG22  | 1:A:26:ALA:HB1   | 1.61                     | 0.81              |
| 1:B:165:GLN:NE2  | 1:B:165:GLN:N    | 2.28                     | 0.81              |
| 1:B:163:GLN:HB3  | 1:B:165:GLN:NE2  | 1.95                     | 0.81              |
| 1:C:163:GLN:HB3  | 1:C:165:GLN:HE22 | 1.45                     | 0.79              |
| 1:D:165:GLN:H    | 1:D:165:GLN:HE21 | 1.30                     | 0.78              |
| 1:C:176:GLU:OE2  | 1:C:179:GLY:HA2  | 1.84                     | 0.78              |
| 1:A:176:GLU:HG3  | 1:A:180:LYS:O    | 1.85                     | 0.77              |
| 1:C:176:GLU:HG3  | 1:C:180:LYS:O    | 1.84                     | 0.77              |
| 2:M:361:HIS:H    | 2:M:361:HIS:CD2  | 2.01                     | 0.77              |
| 2:M:497:ASN:HD22 | 2:M:499:GLU:H    | 1.31                     | 0.77              |
| 1:B:19:ILE:HG22  | 1:B:26:ALA:HB1   | 1.66                     | 0.77              |
| 2:Q:497:ASN:HD22 | 2:Q:499:GLU:H    | 1.32                     | 0.77              |
| 1:B:64:ARG:NH1   | 1:B:100:ASP:O    | 2.18                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:364:LEU:CD2  | 2:P:440:ARG:HD3  | 2.15                     | 0.76              |
| 1:F:49:ILE:HA    | 1:F:180:LYS:HE2  | 1.69                     | 0.75              |
| 2:P:361:HIS:H    | 2:P:361:HIS:CD2  | 2.05                     | 0.75              |
| 2:P:497:ASN:HD22 | 2:P:499:GLU:H    | 1.34                     | 0.74              |
| 2:O:390:LYS:HE2  | 6:O:862:HOH:O    | 1.88                     | 0.73              |
| 2:R:411:LYS:O    | 2:R:414:ARG:NH2  | 2.20                     | 0.73              |
| 2:M:364:LEU:HD22 | 2:M:440:ARG:CD   | 2.19                     | 0.72              |
| 1:E:24:GLU:HG3   | 6:E:781:HOH:O    | 1.89                     | 0.72              |
| 1:F:131:PHE:CD2  | 2:R:475:ILE:HD12 | 2.24                     | 0.72              |
| 1:F:98:THR:OG1   | 1:F:102:GLY:N    | 2.23                     | 0.72              |
| 1:F:24:GLU:HG3   | 6:F:781:HOH:O    | 1.88                     | 0.72              |
| 2:R:416:LEU:C    | 2:R:416:LEU:HD23 | 2.15                     | 0.71              |
| 1:B:24:GLU:HG3   | 6:B:781:HOH:O    | 1.91                     | 0.71              |
| 1:B:165:GLN:H    | 1:B:165:GLN:CD   | 1.95                     | 0.71              |
| 2:Q:361:HIS:H    | 2:Q:361:HIS:HD2  | 1.33                     | 0.71              |
| 1:B:165:GLN:H    | 1:B:165:GLN:HE21 | 1.37                     | 0.71              |
| 1:C:165:GLN:NE2  | 1:C:165:GLN:H    | 1.89                     | 0.71              |
| 2:Q:390:LYS:HD2  | 6:Q:668:HOH:O    | 1.89                     | 0.71              |
| 1:C:24:GLU:HG3   | 6:C:781:HOH:O    | 1.92                     | 0.70              |
| 1:D:24:GLU:HG3   | 6:D:781:HOH:O    | 1.92                     | 0.70              |
| 1:F:180:LYS:HG2  | 1:F:181:THR:N    | 2.06                     | 0.70              |
| 2:N:497:ASN:HD22 | 2:N:499:GLU:H    | 1.39                     | 0.70              |
| 2:R:505:ILE:HG22 | 2:R:507:LYS:HE3  | 1.73                     | 0.70              |
| 1:A:176:GLU:OE2  | 1:A:179:GLY:HA2  | 1.91                     | 0.70              |
| 1:A:24:GLU:HG3   | 6:A:663:HOH:O    | 1.91                     | 0.69              |
| 2:P:497:ASN:ND2  | 2:P:499:GLU:H    | 1.90                     | 0.69              |
| 2:P:361:HIS:H    | 2:P:361:HIS:HD2  | 1.39                     | 0.69              |
| 1:D:98:THR:OG1   | 1:D:102:GLY:N    | 2.24                     | 0.69              |
| 2:M:497:ASN:HD22 | 2:M:497:ASN:C    | 2.00                     | 0.69              |
| 1:D:131:PHE:CD2  | 2:P:475:ILE:HD12 | 2.28                     | 0.69              |
| 2:P:307:ARG:HG2  | 2:P:533:THR:HG22 | 1.74                     | 0.69              |
| 2:M:315:TRP:HZ2  | 2:M:503:GLN:HE21 | 1.40                     | 0.68              |
| 1:E:176:GLU:OE2  | 1:E:179:GLY:HA2  | 1.93                     | 0.68              |
| 1:D:176:GLU:HG3  | 1:D:180:LYS:O    | 1.94                     | 0.68              |
| 2:Q:497:ASN:ND2  | 2:Q:499:GLU:H    | 1.92                     | 0.68              |
| 1:F:176:GLU:OE2  | 1:F:179:GLY:HA2  | 1.94                     | 0.68              |
| 2:Q:315:TRP:HZ2  | 2:Q:503:GLN:HE21 | 1.43                     | 0.67              |
| 1:E:143:LEU:HD23 | 1:E:143:LEU:C    | 2.19                     | 0.67              |
| 1:B:165:GLN:N    | 1:B:165:GLN:HE21 | 1.90                     | 0.66              |
| 2:Q:361:HIS:CG   | 4:Q:601:BME:H21  | 2.30                     | 0.66              |
| 1:C:78:GLU:HG2   | 2:O:301:PRO:CG   | 2.26                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:19:ILE:O     | 2:P:426:VAL:HG21 | 1.95                     | 0.66              |
| 1:B:176:GLU:HG3  | 1:B:180:LYS:C    | 2.21                     | 0.66              |
| 2:M:446:PRO:HD2  | 2:P:376:GLU:HG2  | 1.78                     | 0.65              |
| 2:M:497:ASN:HD22 | 2:M:498:PRO:N    | 1.94                     | 0.65              |
| 2:O:416:LEU:C    | 2:O:416:LEU:HD23 | 2.21                     | 0.65              |
| 2:O:361:HIS:H    | 2:O:361:HIS:CD2  | 2.14                     | 0.65              |
| 1:F:48:HIS:HA    | 1:F:109:VAL:HG12 | 1.77                     | 0.65              |
| 2:R:497:ASN:ND2  | 2:R:499:GLU:OE1  | 2.27                     | 0.65              |
| 2:O:497:ASN:HD22 | 2:O:499:GLU:H    | 1.46                     | 0.64              |
| 2:R:361:HIS:H    | 2:R:361:HIS:HD2  | 1.40                     | 0.64              |
| 1:E:64:ARG:HG2   | 1:E:64:ARG:HH11  | 1.62                     | 0.64              |
| 2:M:361:HIS:H    | 2:M:361:HIS:HD2  | 1.40                     | 0.63              |
| 1:A:163:GLN:HB3  | 1:A:165:GLN:HE22 | 1.63                     | 0.63              |
| 2:R:326:THR:HG22 | 2:R:330:ARG:HD2  | 1.79                     | 0.63              |
| 1:C:131:PHE:O    | 1:C:132:ALA:HB2  | 1.98                     | 0.63              |
| 1:E:19:ILE:O     | 2:Q:426:VAL:HG21 | 1.98                     | 0.63              |
| 2:O:356:PHE:CD2  | 2:O:428:ARG:HD3  | 2.34                     | 0.63              |
| 2:N:361:HIS:CD2  | 2:N:361:HIS:H    | 2.16                     | 0.62              |
| 2:R:406:GLY:O    | 2:R:447:TYR:HD2  | 1.81                     | 0.62              |
| 2:O:361:HIS:CG   | 4:O:601:BME:H21  | 2.35                     | 0.62              |
| 2:M:497:ASN:ND2  | 2:M:499:GLU:N    | 2.45                     | 0.62              |
| 1:E:176:GLU:HG3  | 1:E:180:LYS:O    | 2.00                     | 0.62              |
| 2:R:416:LEU:HD23 | 2:R:417:ALA:N    | 2.14                     | 0.62              |
| 2:R:497:ASN:HD22 | 2:R:497:ASN:C    | 2.07                     | 0.62              |
| 2:O:497:ASN:ND2  | 2:O:499:GLU:H    | 1.97                     | 0.62              |
| 1:D:24:GLU:OE1   | 1:D:25:ALA:N     | 2.30                     | 0.61              |
| 1:F:155:CYS:O    | 1:F:159:ASN:ND2  | 2.33                     | 0.61              |
| 1:E:98:THR:O     | 1:E:102:GLY:HA2  | 2.01                     | 0.60              |
| 2:Q:406:GLY:O    | 2:Q:447:TYR:HD1  | 1.85                     | 0.60              |
| 1:F:49:ILE:CA    | 1:F:180:LYS:HE2  | 2.30                     | 0.60              |
| 1:C:78:GLU:CG    | 2:O:301:PRO:HG2  | 2.30                     | 0.60              |
| 2:O:406:GLY:O    | 2:O:447:TYR:HD1  | 1.84                     | 0.60              |
| 1:B:114:VAL:HG23 | 1:B:122:MET:HE3  | 1.84                     | 0.60              |
| 2:Q:438:SER:O    | 4:Q:601:BME:H22  | 2.02                     | 0.60              |
| 1:B:70:VAL:HG11  | 1:B:106:LEU:HD11 | 1.83                     | 0.60              |
| 2:N:307:ARG:HG2  | 2:N:533:THR:HG22 | 1.83                     | 0.59              |
| 2:O:326:THR:HG22 | 2:O:326:THR:O    | 2.02                     | 0.59              |
| 1:E:131:PHE:CE2  | 1:E:138:HIS:HB3  | 2.37                     | 0.59              |
| 2:M:376:GLU:OE1  | 6:M:639:HOH:O    | 2.16                     | 0.59              |
| 1:B:70:VAL:HG11  | 1:B:106:LEU:CD1  | 2.33                     | 0.59              |
| 1:D:165:GLN:H    | 1:D:165:GLN:NE2  | 1.98                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:376:GLU:O    | 2:P:442:ILE:HA   | 2.03                     | 0.59              |
| 1:F:70:VAL:HG11  | 1:F:106:LEU:HD11 | 1.83                     | 0.59              |
| 1:A:165:GLN:CD   | 1:A:165:GLN:H    | 2.10                     | 0.59              |
| 1:B:78:GLU:HG2   | 2:N:301:PRO:CG   | 2.33                     | 0.59              |
| 1:E:132:ALA:HB3  | 1:E:135:ILE:HD12 | 1.84                     | 0.59              |
| 1:D:153:ALA:HB3  | 1:D:154:LYS:HE3  | 1.84                     | 0.59              |
| 1:D:77:GLY:O     | 1:D:114:VAL:HG12 | 2.03                     | 0.58              |
| 1:A:65:ASP:OD2   | 1:A:133:ARG:HD3  | 2.03                     | 0.58              |
| 2:R:473:LYS:HD2  | 2:R:474:LEU:N    | 2.18                     | 0.58              |
| 1:C:54:GLN:HG3   | 1:C:184:ARG:NH2  | 2.19                     | 0.58              |
| 1:C:165:GLN:H    | 1:C:165:GLN:CD   | 2.10                     | 0.58              |
| 1:B:98:THR:O     | 1:B:102:GLY:HA2  | 2.03                     | 0.58              |
| 1:E:131:PHE:CD2  | 1:E:138:HIS:HB3  | 2.39                     | 0.58              |
| 2:N:326:THR:HG22 | 2:N:330:ARG:HD2  | 1.86                     | 0.58              |
| 1:B:3:GLU:HA     | 1:B:3:GLU:OE1    | 2.03                     | 0.57              |
| 1:F:98:THR:O     | 1:F:102:GLY:HA2  | 2.04                     | 0.57              |
| 1:F:50:LEU:O     | 1:F:182:ALA:HA   | 2.05                     | 0.57              |
| 2:M:406:GLY:O    | 2:M:447:TYR:HD2  | 1.88                     | 0.57              |
| 1:F:176:GLU:HG3  | 1:F:180:LYS:C    | 2.28                     | 0.57              |
| 1:B:78:GLU:HG2   | 2:N:301:PRO:HG3  | 1.86                     | 0.57              |
| 2:P:484:PRO:O    | 2:P:488:MET:HE3  | 2.04                     | 0.57              |
| 1:C:98:THR:O     | 1:C:102:GLY:HA2  | 2.05                     | 0.57              |
| 2:O:356:PHE:CE2  | 2:O:428:ARG:HD3  | 2.40                     | 0.57              |
| 2:R:400:TRP:HA   | 2:R:425:GLY:O    | 2.04                     | 0.57              |
| 1:A:168:GLU:HA   | 1:A:171:ILE:HD12 | 1.87                     | 0.57              |
| 2:M:315:TRP:HZ2  | 2:M:503:GLN:NE2  | 2.01                     | 0.57              |
| 2:N:497:ASN:ND2  | 2:N:499:GLU:H    | 2.03                     | 0.57              |
| 2:M:390:LYS:HD2  | 6:M:644:HOH:O    | 2.05                     | 0.56              |
| 1:C:99:PHE:HE2   | 2:O:411:LYS:HD2  | 1.70                     | 0.56              |
| 1:F:19:ILE:HG22  | 1:F:26:ALA:HB1   | 1.86                     | 0.56              |
| 1:B:131:PHE:CD2  | 1:B:138:HIS:HB3  | 2.40                     | 0.56              |
| 2:P:406:GLY:O    | 2:P:447:TYR:HD1  | 1.89                     | 0.56              |
| 2:P:497:ASN:HD22 | 2:P:497:ASN:C    | 2.14                     | 0.56              |
| 2:P:497:ASN:ND2  | 2:P:499:GLU:HB2  | 2.19                     | 0.56              |
| 1:B:39:LEU:HD11  | 1:B:93:GLY:HA3   | 1.88                     | 0.56              |
| 1:C:98:THR:OG1   | 1:C:102:GLY:N    | 2.38                     | 0.55              |
| 1:F:131:PHE:CE2  | 2:R:475:ILE:HD12 | 2.41                     | 0.55              |
| 2:R:415:TYR:CE1  | 2:R:416:LEU:HD22 | 2.40                     | 0.55              |
| 1:F:19:ILE:O     | 2:R:426:VAL:HG21 | 2.06                     | 0.55              |
| 1:C:19:ILE:O     | 2:O:426:VAL:HG21 | 2.07                     | 0.55              |
| 2:O:497:ASN:HD22 | 2:O:497:ASN:C    | 2.15                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:383:ARG:HD2  | 2:R:436:TYR:CZ   | 2.41                     | 0.55              |
| 2:R:497:ASN:HD22 | 2:R:498:PRO:N    | 2.03                     | 0.55              |
| 1:B:163:GLN:CB   | 1:B:165:GLN:HE22 | 2.17                     | 0.55              |
| 1:A:98:THR:HB    | 1:A:100:ASP:OD1  | 2.07                     | 0.55              |
| 2:Q:497:ASN:ND2  | 2:Q:499:GLU:OE1  | 2.34                     | 0.55              |
| 1:F:24:GLU:OE1   | 1:F:25:ALA:N     | 2.39                     | 0.55              |
| 2:Q:359:HIS:O    | 2:Q:366:ASN:HB3  | 2.06                     | 0.54              |
| 1:A:15:PRO:HB3   | 1:A:133:ARG:HD2  | 1.90                     | 0.54              |
| 1:C:78:GLU:HG2   | 2:O:301:PRO:HG2  | 1.87                     | 0.54              |
| 1:C:114:VAL:HG23 | 1:C:122:MET:HE3  | 1.89                     | 0.54              |
| 1:D:143:LEU:C    | 1:D:143:LEU:HD23 | 2.33                     | 0.54              |
| 2:Q:376:GLU:O    | 2:Q:442:ILE:HA   | 2.07                     | 0.54              |
| 1:C:24:GLU:OE1   | 1:C:25:ALA:N     | 2.37                     | 0.54              |
| 1:D:50:LEU:O     | 1:D:182:ALA:HA   | 2.08                     | 0.54              |
| 2:M:416:LEU:C    | 2:M:416:LEU:CD2  | 2.81                     | 0.54              |
| 2:N:361:HIS:H    | 2:N:361:HIS:HD2  | 1.54                     | 0.54              |
| 1:A:134:GLY:HA3  | 2:M:326:THR:CG2  | 2.36                     | 0.54              |
| 1:C:100:ASP:N    | 1:C:100:ASP:OD1  | 2.40                     | 0.54              |
| 1:A:39:LEU:HD11  | 1:A:93:GLY:HA3   | 1.90                     | 0.54              |
| 1:C:3:GLU:OE1    | 1:C:3:GLU:HA     | 2.07                     | 0.54              |
| 2:R:399:MET:HA   | 2:R:462:HIS:O    | 2.08                     | 0.54              |
| 1:A:100:ASP:OD1  | 1:A:100:ASP:N    | 2.40                     | 0.54              |
| 1:A:180:LYS:HG2  | 1:A:181:THR:N    | 2.23                     | 0.54              |
| 1:D:100:ASP:OD1  | 1:D:100:ASP:N    | 2.40                     | 0.54              |
| 1:C:41:LYS:HD2   | 1:C:88:ALA:HA    | 1.89                     | 0.53              |
| 1:B:50:LEU:O     | 1:B:182:ALA:HA   | 2.08                     | 0.53              |
| 2:N:400:TRP:HA   | 2:N:425:GLY:O    | 2.08                     | 0.53              |
| 1:C:65:ASP:OD2   | 1:C:133:ARG:HD3  | 2.08                     | 0.53              |
| 1:B:69:GLU:HG2   | 1:B:94:ARG:HG2   | 1.90                     | 0.53              |
| 2:N:497:ASN:ND2  | 2:N:499:GLU:HB2  | 2.23                     | 0.53              |
| 1:E:163:GLN:HB3  | 1:E:165:GLN:NE2  | 2.24                     | 0.53              |
| 1:A:19:ILE:HG22  | 1:A:26:ALA:CB    | 2.33                     | 0.53              |
| 2:R:497:ASN:HD22 | 2:R:499:GLU:N    | 1.99                     | 0.53              |
| 1:A:163:GLN:HB3  | 1:A:165:GLN:HE21 | 1.69                     | 0.53              |
| 1:C:39:LEU:HD11  | 1:C:93:GLY:HA3   | 1.90                     | 0.53              |
| 2:M:376:GLU:HG2  | 2:P:446:PRO:HD2  | 1.90                     | 0.53              |
| 1:F:131:PHE:O    | 1:F:132:ALA:HB2  | 2.08                     | 0.53              |
| 2:M:359:HIS:O    | 2:M:366:ASN:HB3  | 2.10                     | 0.52              |
| 2:Q:497:ASN:HD22 | 2:Q:499:GLU:N    | 2.04                     | 0.52              |
| 2:M:335:ALA:HB2  | 2:O:328:ILE:HD12 | 1.90                     | 0.52              |
| 1:B:19:ILE:HD11  | 2:N:408:TYR:HD1  | 1.74                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:406:GLY:O    | 2:N:447:TYR:HD1  | 1.93                     | 0.52              |
| 2:P:400:TRP:HA   | 2:P:425:GLY:O    | 2.09                     | 0.52              |
| 2:R:522:ARG:NE   | 2:R:524:ASP:OD1  | 2.38                     | 0.52              |
| 1:B:143:LEU:C    | 1:B:143:LEU:HD23 | 2.34                     | 0.52              |
| 2:O:326:THR:HG22 | 2:O:330:ARG:HD2  | 1.90                     | 0.52              |
| 2:R:390:LYS:HG2  | 6:R:861:HOH:O    | 2.09                     | 0.52              |
| 2:P:478:LEU:C    | 2:P:478:LEU:HD23 | 2.34                     | 0.52              |
| 2:Q:361:HIS:CD2  | 2:Q:361:HIS:N    | 2.67                     | 0.52              |
| 1:A:176:GLU:HG3  | 1:A:180:LYS:C    | 2.34                     | 0.52              |
| 2:M:363:LEU:HD23 | 2:M:425:GLY:HA2  | 1.90                     | 0.52              |
| 1:C:163:GLN:CB   | 1:C:165:GLN:HE22 | 2.20                     | 0.52              |
| 1:D:147:ASP:OD2  | 1:D:174:ARG:NH1  | 2.42                     | 0.52              |
| 2:R:486:ILE:HB   | 2:R:487:PRO:HD3  | 1.92                     | 0.52              |
| 1:A:35:ILE:HD13  | 2:M:351:PHE:CE1  | 2.45                     | 0.52              |
| 1:C:176:GLU:HG3  | 1:C:180:LYS:C    | 2.35                     | 0.52              |
| 2:P:386:ASP:HA   | 2:P:527:LEU:O    | 2.10                     | 0.52              |
| 1:A:19:ILE:HG21  | 2:M:410:HIS:HB2  | 1.92                     | 0.52              |
| 1:A:78:GLU:HG2   | 2:M:301:PRO:HB3  | 1.91                     | 0.52              |
| 2:M:390:LYS:CD   | 6:M:644:HOH:O    | 2.58                     | 0.52              |
| 2:N:416:LEU:HD23 | 2:N:416:LEU:C    | 2.35                     | 0.52              |
| 2:R:376:GLU:O    | 2:R:442:ILE:HA   | 2.10                     | 0.52              |
| 1:A:143:LEU:C    | 1:A:143:LEU:HD23 | 2.34                     | 0.51              |
| 2:M:364:LEU:CD2  | 2:M:440:ARG:HD3  | 2.34                     | 0.51              |
| 2:Q:362:ASP:OD1  | 2:Q:440:ARG:HD3  | 2.09                     | 0.51              |
| 2:M:360:ASP:OD2  | 2:M:428:ARG:HD2  | 2.10                     | 0.51              |
| 2:N:488:MET:CE   | 1:C:1:PRO:HG3    | 2.40                     | 0.51              |
| 1:D:155:CYS:HB3  | 1:D:158:LEU:HB2  | 1.91                     | 0.51              |
| 2:R:536:GLU:HB2  | 6:R:840:HOH:O    | 2.10                     | 0.51              |
| 2:N:359:HIS:O    | 2:N:366:ASN:HB3  | 2.10                     | 0.51              |
| 2:M:448:PRO:HB2  | 2:P:516:MET:HA   | 1.92                     | 0.51              |
| 1:E:29:PRO:O     | 6:E:807:HOH:O    | 2.19                     | 0.51              |
| 1:B:20:GLY:C     | 1:B:21:LEU:HD23  | 2.36                     | 0.51              |
| 1:D:78:GLU:CG    | 2:P:301:PRO:CG   | 2.89                     | 0.51              |
| 1:D:176:GLU:HA   | 1:D:180:LYS:O    | 2.10                     | 0.51              |
| 1:E:64:ARG:NH1   | 1:E:64:ARG:HG2   | 2.23                     | 0.51              |
| 2:R:505:ILE:HG22 | 2:R:507:LYS:CE   | 2.38                     | 0.51              |
| 1:F:36:TRP:CG    | 1:F:37:ASN:H     | 2.29                     | 0.51              |
| 2:M:405:GLY:HA3  | 6:M:647:HOH:O    | 2.11                     | 0.51              |
| 2:M:356:PHE:CD1  | 2:M:428:ARG:HD3  | 2.46                     | 0.50              |
| 1:F:70:VAL:HG11  | 1:F:106:LEU:CD1  | 2.41                     | 0.50              |
| 2:R:361:HIS:CD2  | 2:R:361:HIS:N    | 2.69                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:36:TRP:CG    | 1:C:37:ASN:H     | 2.29                     | 0.50              |
| 2:O:356:PHE:HD2  | 2:O:428:ARG:CD   | 2.24                     | 0.50              |
| 2:Q:394:ASN:O    | 6:Q:643:HOH:O    | 2.20                     | 0.50              |
| 2:R:497:ASN:ND2  | 2:R:499:GLU:N    | 2.47                     | 0.50              |
| 2:O:478:LEU:HD23 | 2:O:478:LEU:C    | 2.37                     | 0.50              |
| 2:P:364:LEU:HD11 | 2:P:442:ILE:HG23 | 1.93                     | 0.50              |
| 2:M:497:ASN:ND2  | 2:M:497:ASN:C    | 2.70                     | 0.50              |
| 1:C:180:LYS:HG2  | 1:C:181:THR:N    | 2.27                     | 0.50              |
| 2:P:359:HIS:O    | 2:P:366:ASN:HB3  | 2.11                     | 0.50              |
| 2:M:306:SER:OG   | 2:M:530:GLN:NE2  | 2.35                     | 0.50              |
| 2:O:382:GLY:HA3  | 2:O:523:PHE:O    | 2.12                     | 0.50              |
| 2:P:390:LYS:HD2  | 6:P:682:HOH:O    | 2.11                     | 0.50              |
| 2:P:497:ASN:HD22 | 2:P:499:GLU:N    | 2.08                     | 0.50              |
| 1:B:114:VAL:HG23 | 1:B:122:MET:CE   | 2.41                     | 0.50              |
| 2:Q:416:LEU:HD23 | 2:Q:416:LEU:C    | 2.35                     | 0.50              |
| 1:F:144:TYR:CE2  | 1:F:158:LEU:HD22 | 2.46                     | 0.50              |
| 2:O:326:THR:CG2  | 2:O:330:ARG:HD2  | 2.42                     | 0.50              |
| 1:D:131:PHE:CD2  | 1:D:138:HIS:HB3  | 2.47                     | 0.50              |
| 2:M:362:ASP:OD1  | 2:M:440:ARG:HD2  | 2.11                     | 0.49              |
| 2:Q:497:ASN:ND2  | 2:Q:499:GLU:HB2  | 2.27                     | 0.49              |
| 1:B:180:LYS:HG2  | 1:B:181:THR:N    | 2.27                     | 0.49              |
| 1:C:143:LEU:HD23 | 1:C:143:LEU:C    | 2.37                     | 0.49              |
| 1:C:176:GLU:OE2  | 1:C:179:GLY:CA   | 2.58                     | 0.49              |
| 2:P:497:ASN:HD21 | 2:P:499:GLU:HB2  | 1.77                     | 0.49              |
| 2:P:486:ILE:HB   | 2:P:487:PRO:HD3  | 1.94                     | 0.49              |
| 2:R:405:GLY:HA3  | 6:R:787:HOH:O    | 2.13                     | 0.49              |
| 1:A:114:VAL:HG23 | 1:A:122:MET:HE3  | 1.93                     | 0.49              |
| 1:B:20:GLY:O     | 1:B:21:LEU:HD23  | 2.12                     | 0.49              |
| 2:R:315:TRP:HZ2  | 2:R:503:GLN:HE21 | 1.60                     | 0.49              |
| 2:O:390:LYS:HD3  | 6:O:784:HOH:O    | 2.11                     | 0.49              |
| 1:D:33:GLN:O     | 2:P:428:ARG:NH2  | 2.43                     | 0.49              |
| 2:P:326:THR:O    | 2:P:326:THR:HG22 | 2.12                     | 0.49              |
| 1:F:31:ARG:NH1   | 2:R:428:ARG:HG2  | 2.28                     | 0.49              |
| 1:F:69:GLU:HG2   | 1:F:94:ARG:HG2   | 1.95                     | 0.49              |
| 2:M:376:GLU:O    | 2:M:442:ILE:HA   | 2.13                     | 0.49              |
| 1:E:176:GLU:HA   | 1:E:180:LYS:O    | 2.13                     | 0.49              |
| 2:R:437:TYR:CD1  | 2:R:437:TYR:C    | 2.91                     | 0.49              |
| 1:C:163:GLN:HB3  | 1:C:165:GLN:HE21 | 1.72                     | 0.48              |
| 2:O:399:MET:HA   | 2:O:462:HIS:O    | 2.12                     | 0.48              |
| 2:M:315:TRP:CZ2  | 2:M:503:GLN:NE2  | 2.80                     | 0.48              |
| 2:M:356:PHE:HD1  | 2:M:428:ARG:HD3  | 1.78                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:24:GLU:OE1   | 1:E:25:ALA:N     | 2.46                     | 0.48              |
| 2:M:434:ASP:HB3  | 2:M:436:TYR:CD2  | 2.48                     | 0.48              |
| 2:M:484:PRO:O    | 2:M:488:MET:HE3  | 2.12                     | 0.48              |
| 2:O:400:TRP:HA   | 2:O:425:GLY:O    | 2.13                     | 0.48              |
| 1:E:70:VAL:HG11  | 1:E:106:LEU:HD11 | 1.95                     | 0.48              |
| 1:A:20:GLY:C     | 1:A:21:LEU:HD23  | 2.38                     | 0.48              |
| 2:Q:362:ASP:OD1  | 2:Q:440:ARG:CD   | 2.62                     | 0.48              |
| 1:A:50:LEU:O     | 1:A:182:ALA:HA   | 2.12                     | 0.48              |
| 2:N:361:HIS:ND1  | 4:N:601:BME:H21  | 2.29                     | 0.48              |
| 1:F:84:ASN:OD1   | 1:F:86:GLU:HB2   | 2.13                     | 0.48              |
| 1:E:70:VAL:HG12  | 1:E:128:ILE:HG12 | 1.95                     | 0.48              |
| 1:A:114:VAL:CG2  | 1:A:122:MET:HE3  | 2.44                     | 0.48              |
| 2:M:307:ARG:HG2  | 2:M:533:THR:HG22 | 1.95                     | 0.48              |
| 2:M:497:ASN:HD22 | 2:M:499:GLU:N    | 2.05                     | 0.48              |
| 2:O:356:PHE:CD2  | 2:O:428:ARG:CD   | 2.97                     | 0.48              |
| 1:F:33:GLN:HG2   | 1:F:85:LEU:HD12  | 1.95                     | 0.48              |
| 1:E:176:GLU:HG3  | 1:E:180:LYS:C    | 2.39                     | 0.48              |
| 2:M:364:LEU:HB2  | 2:M:440:ARG:HD3  | 1.96                     | 0.48              |
| 1:C:11:GLN:HB2   | 2:O:477:GLN:HG3  | 1.96                     | 0.47              |
| 1:D:28:ASN:HB3   | 1:D:29:PRO:HD2   | 1.96                     | 0.47              |
| 2:P:372:LEU:HA   | 2:P:373:PRO:HD3  | 1.83                     | 0.47              |
| 1:F:18:HIS:CE1   | 1:F:99:PHE:HE1   | 2.32                     | 0.47              |
| 1:F:171:ILE:HD12 | 1:F:171:ILE:H    | 1.78                     | 0.47              |
| 2:M:508:LEU:HD23 | 2:P:488:MET:HE1  | 1.95                     | 0.47              |
| 1:B:176:GLU:OE2  | 1:B:179:GLY:C    | 2.57                     | 0.47              |
| 1:F:171:ILE:HD12 | 1:F:171:ILE:N    | 2.29                     | 0.47              |
| 2:R:488:MET:C    | 2:R:493:LYS:HE2  | 2.39                     | 0.47              |
| 1:B:132:ALA:HB3  | 1:B:135:ILE:HD12 | 1.95                     | 0.47              |
| 1:D:176:GLU:HG3  | 1:D:180:LYS:C    | 2.38                     | 0.47              |
| 2:Q:399:MET:HA   | 2:Q:462:HIS:O    | 2.14                     | 0.47              |
| 1:F:176:GLU:OE2  | 1:F:179:GLY:CA   | 2.61                     | 0.47              |
| 2:R:356:PHE:CD1  | 2:R:428:ARG:HD3  | 2.49                     | 0.47              |
| 1:A:132:ALA:HB3  | 1:A:135:ILE:HD12 | 1.95                     | 0.47              |
| 1:A:176:GLU:OE2  | 1:A:179:GLY:CA   | 2.61                     | 0.47              |
| 2:M:316:HIS:HB3  | 2:M:317:PRO:HD2  | 1.95                     | 0.47              |
| 2:M:383:ARG:NH2  | 2:M:434:ASP:OD1  | 2.47                     | 0.47              |
| 1:B:78:GLU:CG    | 2:N:301:PRO:CG   | 2.93                     | 0.47              |
| 1:C:18:HIS:CE1   | 1:C:99:PHE:HE1   | 2.32                     | 0.47              |
| 2:O:385:VAL:O    | 2:O:526:VAL:HA   | 2.14                     | 0.47              |
| 1:D:72:GLN:O     | 1:D:91:SER:OG    | 2.33                     | 0.47              |
| 2:Q:364:LEU:HB2  | 2:Q:440:ARG:HD3  | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:453:PRO:HB2  | 2:R:310:ILE:HD12 | 1.96                     | 0.47              |
| 2:R:383:ARG:NH2  | 2:R:391:PRO:HG3  | 2.30                     | 0.47              |
| 1:B:131:PHE:CE2  | 1:B:138:HIS:HB3  | 2.50                     | 0.47              |
| 1:D:15:PRO:HB3   | 1:D:133:ARG:HD2  | 1.96                     | 0.47              |
| 1:F:99:PHE:HE2   | 2:R:411:LYS:HD2  | 1.80                     | 0.47              |
| 2:M:350:ASN:C    | 2:M:350:ASN:OD1  | 2.57                     | 0.47              |
| 1:C:19:ILE:HD11  | 2:O:408:TYR:HD2  | 1.79                     | 0.47              |
| 2:O:326:THR:O    | 2:O:326:THR:CG2  | 2.63                     | 0.47              |
| 1:E:165:GLN:H    | 1:E:165:GLN:HE21 | 0.65                     | 0.47              |
| 1:F:100:ASP:OD1  | 1:F:100:ASP:N    | 2.47                     | 0.47              |
| 1:A:176:GLU:HA   | 1:A:180:LYS:O    | 2.15                     | 0.47              |
| 2:M:489:CYS:O    | 2:M:493:LYS:HE3  | 2.14                     | 0.47              |
| 1:D:51:LEU:O     | 1:D:105:THR:HA   | 2.14                     | 0.47              |
| 1:C:176:GLU:HA   | 1:C:180:LYS:O    | 2.15                     | 0.46              |
| 2:P:405:GLY:HA3  | 6:P:685:HOH:O    | 2.15                     | 0.46              |
| 1:F:176:GLU:OE2  | 1:F:179:GLY:C    | 2.58                     | 0.46              |
| 1:A:25:ALA:O     | 2:M:411:LYS:NZ   | 2.48                     | 0.46              |
| 2:R:416:LEU:C    | 2:R:416:LEU:CD2  | 2.88                     | 0.46              |
| 1:F:39:LEU:HD11  | 1:F:93:GLY:HA3   | 1.98                     | 0.46              |
| 2:R:489:CYS:HA   | 2:R:490:PRO:HD3  | 1.69                     | 0.46              |
| 1:A:19:ILE:HG23  | 2:M:410:HIS:HD2  | 1.79                     | 0.46              |
| 2:O:420:ASP:HA   | 2:O:421:PRO:HD2  | 1.73                     | 0.46              |
| 2:Q:416:LEU:HD23 | 2:Q:417:ALA:N    | 2.29                     | 0.46              |
| 2:R:315:TRP:HZ2  | 2:R:503:GLN:NE2  | 2.14                     | 0.46              |
| 1:A:98:THR:O     | 1:A:102:GLY:HA2  | 2.15                     | 0.46              |
| 1:E:98:THR:HB    | 1:E:100:ASP:OD1  | 2.15                     | 0.46              |
| 1:A:24:GLU:OE1   | 1:A:25:ALA:N     | 2.46                     | 0.46              |
| 1:E:165:GLN:NE2  | 1:E:165:GLN:N    | 2.30                     | 0.46              |
| 2:M:478:LEU:HD23 | 2:M:478:LEU:C    | 2.41                     | 0.46              |
| 1:C:50:LEU:O     | 1:C:182:ALA:HA   | 2.15                     | 0.46              |
| 1:F:35:ILE:HD13  | 2:R:351:PHE:CE1  | 2.50                     | 0.46              |
| 1:F:131:PHE:CE2  | 1:F:138:HIS:HB3  | 2.51                     | 0.46              |
| 1:F:165:GLN:HE21 | 1:F:165:GLN:N    | 2.02                     | 0.46              |
| 2:M:448:PRO:HD3  | 2:M:456:TRP:CZ3  | 2.51                     | 0.46              |
| 1:E:180:LYS:CG   | 1:E:181:THR:N    | 2.79                     | 0.46              |
| 2:R:478:LEU:C    | 2:R:478:LEU:HD23 | 2.41                     | 0.46              |
| 1:D:153:ALA:CB   | 1:D:154:LYS:HE3  | 2.46                     | 0.45              |
| 1:D:18:HIS:CE1   | 1:D:99:PHE:CE1   | 3.04                     | 0.45              |
| 2:N:497:ASN:HA   | 2:N:498:PRO:HD2  | 1.87                     | 0.45              |
| 1:A:18:HIS:CE1   | 1:A:99:PHE:HE1   | 2.34                     | 0.45              |
| 1:A:70:VAL:HG11  | 1:A:106:LEU:HD11 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:373:PRO:HB3  | 2:N:423:PHE:HB2  | 1.99                     | 0.45              |
| 2:N:497:ASN:HD22 | 2:N:497:ASN:C    | 2.24                     | 0.45              |
| 2:P:360:ASP:OD2  | 2:P:428:ARG:NH1  | 2.42                     | 0.45              |
| 1:E:65:ASP:OD2   | 1:E:133:ARG:HD3  | 2.17                     | 0.45              |
| 2:Q:516:MET:HE3  | 2:Q:516:MET:HB3  | 1.81                     | 0.45              |
| 1:D:163:GLN:HA   | 1:D:164:PRO:HD3  | 1.85                     | 0.45              |
| 1:E:64:ARG:HH11  | 1:E:64:ARG:CG    | 2.23                     | 0.45              |
| 1:E:70:VAL:HG11  | 1:E:106:LEU:CD1  | 2.47                     | 0.45              |
| 1:A:54:GLN:HG2   | 1:A:102:GLY:O    | 2.16                     | 0.45              |
| 2:N:361:HIS:CG   | 4:N:601:BME:H21  | 2.52                     | 0.45              |
| 2:O:489:CYS:HA   | 2:O:490:PRO:HD3  | 1.69                     | 0.45              |
| 2:Q:484:PRO:O    | 2:Q:487:PRO:HD2  | 2.16                     | 0.45              |
| 2:O:315:TRP:HZ2  | 2:O:503:GLN:NE2  | 2.15                     | 0.45              |
| 1:D:18:HIS:CE1   | 1:D:99:PHE:HE1   | 2.35                     | 0.45              |
| 2:Q:364:LEU:HD22 | 2:Q:440:ARG:HD3  | 1.97                     | 0.45              |
| 1:B:190:GLN:HG3  | 2:N:333:ARG:HG2  | 1.99                     | 0.45              |
| 2:N:489:CYS:HA   | 2:N:490:PRO:HD3  | 1.83                     | 0.45              |
| 2:Q:411:LYS:O    | 2:Q:414:ARG:NH2  | 2.43                     | 0.45              |
| 2:O:376:GLU:O    | 2:O:442:ILE:HA   | 2.16                     | 0.44              |
| 1:D:24:GLU:O     | 1:D:27:GLY:N     | 2.45                     | 0.44              |
| 1:F:50:LEU:HD23  | 1:F:177:VAL:HB   | 1.98                     | 0.44              |
| 2:N:478:LEU:C    | 2:N:478:LEU:HD23 | 2.41                     | 0.44              |
| 1:F:115:ASN:HA   | 1:F:121:PRO:HA   | 1.99                     | 0.44              |
| 2:M:495:ILE:CG2  | 2:M:500:ALA:HB3  | 2.47                     | 0.44              |
| 2:Q:315:TRP:CZ2  | 2:Q:503:GLN:NE2  | 2.86                     | 0.44              |
| 2:N:488:MET:C    | 2:N:493:LYS:HE2  | 2.43                     | 0.44              |
| 2:Q:362:ASP:OD1  | 2:Q:364:LEU:HB2  | 2.16                     | 0.44              |
| 1:F:120:VAL:HA   | 1:F:121:PRO:HD3  | 1.81                     | 0.44              |
| 1:A:163:GLN:HA   | 1:A:164:PRO:HD2  | 1.89                     | 0.44              |
| 2:Q:497:ASN:HD22 | 2:Q:497:ASN:C    | 2.25                     | 0.44              |
| 1:E:36:TRP:CG    | 1:E:37:ASN:H     | 2.36                     | 0.44              |
| 2:Q:489:CYS:O    | 2:Q:493:LYS:HE3  | 2.18                     | 0.44              |
| 2:Q:536:GLU:HB2  | 6:Q:722:HOH:O    | 2.17                     | 0.44              |
| 2:R:364:LEU:HB2  | 2:R:440:ARG:HD3  | 1.99                     | 0.44              |
| 1:D:36:TRP:CG    | 1:D:37:ASN:H     | 2.35                     | 0.44              |
| 1:E:41:LYS:HD2   | 1:E:88:ALA:HA    | 1.99                     | 0.44              |
| 2:Q:497:ASN:HD21 | 2:Q:499:GLU:HB2  | 1.83                     | 0.44              |
| 2:O:486:ILE:N    | 2:O:487:PRO:HD2  | 2.33                     | 0.44              |
| 1:D:65:ASP:OD2   | 1:D:133:ARG:HD3  | 2.18                     | 0.44              |
| 1:E:176:GLU:OE2  | 1:E:179:GLY:CA   | 2.63                     | 0.44              |
| 2:Q:405:GLY:HA3  | 6:Q:671:HOH:O    | 2.16                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:416:LEU:C    | 2:O:416:LEU:CD2  | 2.89                     | 0.44              |
| 1:D:131:PHE:CE2  | 1:D:138:HIS:HB3  | 2.53                     | 0.44              |
| 2:Q:315:TRP:HZ2  | 2:Q:503:GLN:NE2  | 2.10                     | 0.44              |
| 1:C:99:PHE:CE2   | 2:O:411:LYS:HD2  | 2.52                     | 0.43              |
| 1:E:84:ASN:O     | 1:E:87:ASN:HB2   | 2.18                     | 0.43              |
| 1:F:65:ASP:OD2   | 1:F:133:ARG:HD3  | 2.18                     | 0.43              |
| 2:R:371:GLY:N    | 2:R:422:ASN:ND2  | 2.66                     | 0.43              |
| 1:E:8:THR:HA     | 1:E:9:PRO:HD3    | 1.85                     | 0.43              |
| 2:Q:415:TYR:CE1  | 2:Q:416:LEU:HD22 | 2.53                     | 0.43              |
| 2:R:434:ASP:HB3  | 2:R:436:TYR:CD2  | 2.53                     | 0.43              |
| 1:A:1:PRO:HG2    | 2:O:488:MET:HE2  | 2.00                     | 0.43              |
| 1:A:131:PHE:CD2  | 1:A:138:HIS:HB3  | 2.54                     | 0.43              |
| 1:B:1:PRO:H3     | 2:P:481:GLU:CD   | 2.26                     | 0.43              |
| 2:O:438:SER:O    | 4:O:601:BME:H22  | 2.19                     | 0.43              |
| 1:E:58:GLY:HA2   | 1:E:190:GLN:HB3  | 2.00                     | 0.43              |
| 1:F:52:LEU:C     | 1:F:52:LEU:HD22  | 2.43                     | 0.43              |
| 2:Q:407:ARG:HD3  | 2:Q:417:ALA:O    | 2.18                     | 0.43              |
| 2:Q:420:ASP:HA   | 2:Q:421:PRO:HD2  | 1.81                     | 0.43              |
| 2:Q:488:MET:CE   | 1:F:1:PRO:HG2    | 2.49                     | 0.43              |
| 2:R:497:ASN:HA   | 2:R:498:PRO:HD3  | 1.76                     | 0.43              |
| 1:A:78:GLU:HG2   | 2:M:301:PRO:CB   | 2.48                     | 0.43              |
| 2:P:489:CYS:C    | 2:P:493:LYS:HE3  | 2.44                     | 0.43              |
| 2:O:315:TRP:HZ2  | 2:O:503:GLN:HE21 | 1.67                     | 0.43              |
| 2:O:390:LYS:HA   | 2:O:391:PRO:HD3  | 1.81                     | 0.43              |
| 1:D:131:PHE:CE2  | 2:P:475:ILE:HD12 | 2.53                     | 0.43              |
| 2:P:519:LEU:HD23 | 2:P:519:LEU:HA   | 1.95                     | 0.43              |
| 1:F:80:GLN:O     | 1:F:91:SER:HB2   | 2.18                     | 0.43              |
| 2:O:489:CYS:C    | 2:O:493:LYS:HE2  | 2.43                     | 0.43              |
| 2:P:350:ASN:OD1  | 2:P:350:ASN:C    | 2.62                     | 0.43              |
| 2:P:376:GLU:OE1  | 6:P:676:HOH:O    | 2.21                     | 0.43              |
| 2:P:390:LYS:HE2  | 6:P:759:HOH:O    | 2.19                     | 0.43              |
| 2:P:307:ARG:HD2  | 6:P:695:HOH:O    | 2.19                     | 0.43              |
| 2:Q:522:ARG:NH1  | 6:Q:690:HOH:O    | 2.51                     | 0.43              |
| 1:F:33:GLN:HB3   | 1:F:85:LEU:HD11  | 2.01                     | 0.43              |
| 1:E:110:LYS:NZ   | 1:E:147:ASP:OD1  | 2.46                     | 0.42              |
| 2:R:326:THR:CG2  | 2:R:330:ARG:HD2  | 2.45                     | 0.42              |
| 2:R:505:ILE:O    | 2:R:507:LYS:HE3  | 2.19                     | 0.42              |
| 1:A:114:VAL:HG23 | 1:A:122:MET:CE   | 2.49                     | 0.42              |
| 2:O:497:ASN:HA   | 2:O:498:PRO:HD2  | 1.90                     | 0.42              |
| 1:C:158:LEU:HD12 | 1:C:158:LEU:HA   | 1.82                     | 0.42              |
| 2:O:359:HIS:O    | 2:O:366:ASN:HB3  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:163:GLN:HG3  | 1:F:61:HIS:ND1   | 2.34                     | 0.42              |
| 1:E:50:LEU:O     | 1:E:182:ALA:HA   | 2.20                     | 0.42              |
| 1:F:51:LEU:O     | 1:F:105:THR:HA   | 2.19                     | 0.42              |
| 1:B:64:ARG:HD3   | 1:B:99:PHE:O     | 2.19                     | 0.42              |
| 1:C:155:CYS:HB3  | 1:C:158:LEU:HB2  | 2.01                     | 0.42              |
| 2:O:495:ILE:CG2  | 2:O:500:ALA:HB3  | 2.50                     | 0.42              |
| 2:Q:364:LEU:HD22 | 2:Q:440:ARG:CD   | 2.48                     | 0.42              |
| 1:F:134:GLY:HA3  | 2:R:326:THR:HG22 | 2.00                     | 0.42              |
| 2:M:489:CYS:HA   | 2:M:490:PRO:HD3  | 1.74                     | 0.42              |
| 2:O:406:GLY:O    | 2:O:447:TYR:CD1  | 2.69                     | 0.42              |
| 2:P:411:LYS:H    | 2:P:411:LYS:HG3  | 1.56                     | 0.42              |
| 1:E:100:ASP:OD1  | 1:E:100:ASP:N    | 2.52                     | 0.42              |
| 1:F:168:GLU:CA   | 1:F:171:ILE:CD1  | 2.83                     | 0.42              |
| 1:A:158:LEU:HD12 | 1:A:158:LEU:HA   | 1.90                     | 0.42              |
| 1:A:165:GLN:NE2  | 1:A:165:GLN:H    | 2.17                     | 0.42              |
| 1:B:168:GLU:HA   | 1:B:171:ILE:HD12 | 2.01                     | 0.42              |
| 2:N:489:CYS:C    | 2:N:493:LYS:HE3  | 2.45                     | 0.42              |
| 1:C:35:ILE:HG21  | 1:C:92:PHE:HE2   | 1.83                     | 0.42              |
| 1:C:52:LEU:C     | 1:C:52:LEU:HD22  | 2.45                     | 0.42              |
| 1:C:52:LEU:CD2   | 1:C:184:ARG:NH1  | 2.82                     | 0.42              |
| 2:P:363:LEU:HD23 | 2:P:425:GLY:HA2  | 2.00                     | 0.42              |
| 2:N:392:VAL:HG12 | 2:N:395:THR:HB   | 2.01                     | 0.42              |
| 1:D:78:GLU:HG2   | 2:P:301:PRO:CG   | 2.50                     | 0.42              |
| 2:P:497:ASN:HA   | 2:P:498:PRO:HD2  | 1.75                     | 0.42              |
| 1:A:110:LYS:NZ   | 1:A:147:ASP:OD1  | 2.53                     | 0.42              |
| 1:B:61:HIS:ND1   | 1:C:163:GLN:HG3  | 2.35                     | 0.42              |
| 2:P:522:ARG:NH1  | 6:P:706:HOH:O    | 2.53                     | 0.42              |
| 1:E:84:ASN:OD1   | 1:E:86:GLU:HB2   | 2.20                     | 0.42              |
| 2:R:378:ILE:HA   | 2:R:519:LEU:O    | 2.20                     | 0.42              |
| 2:M:420:ASP:HA   | 2:M:421:PRO:HD2  | 1.74                     | 0.42              |
| 1:C:131:PHE:O    | 1:C:132:ALA:CB   | 2.65                     | 0.42              |
| 2:O:364:LEU:HD22 | 2:O:440:ARG:CD   | 2.50                     | 0.42              |
| 1:F:33:GLN:CG    | 1:F:85:LEU:HD12  | 2.49                     | 0.42              |
| 1:F:54:GLN:HG3   | 1:F:184:ARG:NH2  | 2.35                     | 0.42              |
| 2:R:307:ARG:NE   | 2:R:536:GLU:OE2  | 2.48                     | 0.42              |
| 2:R:359:HIS:O    | 2:R:366:ASN:HB3  | 2.20                     | 0.42              |
| 1:A:131:PHE:CD2  | 2:M:475:ILE:HD12 | 2.54                     | 0.42              |
| 1:C:31:ARG:HB3   | 6:O:835:HOH:O    | 2.19                     | 0.42              |
| 2:P:510:MET:HE3  | 2:P:510:MET:HB3  | 1.94                     | 0.42              |
| 2:Q:413:ASP:O    | 2:Q:414:ARG:CZ   | 2.68                     | 0.42              |
| 2:Q:522:ARG:NE   | 2:Q:524:ASP:OD1  | 2.50                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:522:ARG:HH11 | 2:R:522:ARG:HD3  | 1.34                     | 0.42              |
| 1:A:176:GLU:OE2  | 1:A:179:GLY:C    | 2.63                     | 0.41              |
| 2:M:497:ASN:HA   | 2:M:498:PRO:HD2  | 1.66                     | 0.41              |
| 2:M:516:MET:HB3  | 2:M:516:MET:HE3  | 1.82                     | 0.41              |
| 2:N:486:ILE:N    | 2:N:487:PRO:HD2  | 2.35                     | 0.41              |
| 1:C:79:TYR:O     | 2:O:301:PRO:HB3  | 2.19                     | 0.41              |
| 2:M:497:ASN:ND2  | 2:M:499:GLU:HB2  | 2.35                     | 0.41              |
| 2:N:399:MET:HA   | 2:N:462:HIS:O    | 2.21                     | 0.41              |
| 1:F:176:GLU:HA   | 1:F:180:LYS:O    | 2.19                     | 0.41              |
| 1:B:70:VAL:CG1   | 1:B:106:LEU:HD11 | 2.50                     | 0.41              |
| 2:O:405:GLY:HA3  | 6:O:787:HOH:O    | 2.19                     | 0.41              |
| 2:P:497:ASN:HD22 | 2:P:498:PRO:N    | 2.18                     | 0.41              |
| 1:E:62:LEU:HD13  | 1:E:101:ALA:O    | 2.20                     | 0.41              |
| 2:M:372:LEU:HA   | 2:M:373:PRO:HD3  | 1.89                     | 0.41              |
| 1:B:120:VAL:HA   | 1:B:121:PRO:HD3  | 1.95                     | 0.41              |
| 2:O:411:LYS:H    | 2:O:411:LYS:HG3  | 1.64                     | 0.41              |
| 1:D:63:VAL:HG12  | 1:D:66:SER:HB3   | 2.03                     | 0.41              |
| 1:D:140:HIS:O    | 1:D:197:PHE:HA   | 2.20                     | 0.41              |
| 1:B:15:PRO:HB3   | 1:B:133:ARG:HD2  | 2.02                     | 0.41              |
| 2:N:405:GLY:HA3  | 6:N:749:HOH:O    | 2.20                     | 0.41              |
| 2:O:356:PHE:HD2  | 2:O:428:ARG:HD2  | 1.84                     | 0.41              |
| 1:F:19:ILE:O     | 2:R:426:VAL:CG2  | 2.67                     | 0.41              |
| 1:B:195:THR:HG22 | 1:B:196:VAL:O    | 2.21                     | 0.41              |
| 2:N:315:TRP:HZ2  | 2:N:503:GLN:HE21 | 1.68                     | 0.41              |
| 2:Q:372:LEU:HA   | 2:Q:373:PRO:HD3  | 1.94                     | 0.41              |
| 2:R:363:LEU:HD12 | 2:R:363:LEU:N    | 2.36                     | 0.41              |
| 2:N:489:CYS:O    | 2:N:493:LYS:HE3  | 2.21                     | 0.41              |
| 2:Q:400:TRP:HA   | 2:Q:425:GLY:O    | 2.21                     | 0.41              |
| 1:F:165:GLN:NE2  | 1:F:165:GLN:N    | 2.50                     | 0.41              |
| 1:B:133:ARG:NH2  | 1:C:162:GLU:OE2  | 2.51                     | 0.41              |
| 2:O:361:HIS:H    | 2:O:361:HIS:HD2  | 1.66                     | 0.41              |
| 1:E:51:LEU:HD11  | 1:E:126:ILE:HD12 | 2.02                     | 0.41              |
| 1:F:99:PHE:CE2   | 2:R:411:LYS:HD2  | 2.55                     | 0.41              |
| 2:M:495:ILE:HG21 | 2:M:500:ALA:HB3  | 2.03                     | 0.41              |
| 2:M:497:ASN:HD21 | 2:M:499:GLU:HB2  | 1.86                     | 0.41              |
| 2:M:500:ALA:O    | 2:M:503:GLN:HB2  | 2.21                     | 0.41              |
| 1:B:163:GLN:C    | 1:B:165:GLN:NE2  | 2.79                     | 0.41              |
| 1:C:24:GLU:CD    | 1:C:25:ALA:H     | 2.29                     | 0.41              |
| 2:R:364:LEU:HD22 | 2:R:440:ARG:HD3  | 2.02                     | 0.41              |
| 1:C:2:ILE:HA     | 1:C:2:ILE:HD13   | 1.83                     | 0.40              |
| 2:P:326:THR:O    | 2:P:326:THR:CG2  | 2.69                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:Q:486:ILE:HB   | 2:Q:487:PRO:HD3 | 2.03                     | 0.40              |
| 2:Q:489:CYS:C    | 2:Q:493:LYS:HE3 | 2.46                     | 0.40              |
| 2:M:361:HIS:CD2  | 2:M:361:HIS:N   | 2.74                     | 0.40              |
| 1:D:180:LYS:HG2  | 1:D:181:THR:N   | 2.36                     | 0.40              |
| 1:F:78:GLU:CG    | 2:R:301:PRO:CG  | 2.99                     | 0.40              |
| 1:F:147:ASP:OD2  | 1:F:174:ARG:NH1 | 2.49                     | 0.40              |
| 2:N:457:ARG:HA   | 2:N:458:PRO:HD3 | 1.93                     | 0.40              |
| 2:R:497:ASN:ND2  | 2:R:497:ASN:C   | 2.78                     | 0.40              |
| 2:R:497:ASN:ND2  | 2:R:499:GLU:HB2 | 2.36                     | 0.40              |
| 1:C:30:THR:HB    | 1:C:34:GLU:HG3  | 2.03                     | 0.40              |
| 1:D:78:GLU:CD    | 2:P:301:PRO:HG2 | 2.47                     | 0.40              |
| 2:P:450:ARG:HG3  | 6:P:673:HOH:O   | 2.21                     | 0.40              |
| 2:O:437:TYR:CD1  | 2:O:437:TYR:C   | 2.98                     | 0.40              |
| 1:F:160:LEU:HD23 | 1:F:160:LEU:HA  | 1.89                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 198/200 (99%) | 193 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | B     | 198/200 (99%) | 192 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | C     | 198/200 (99%) | 190 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 1   | D     | 198/200 (99%) | 189 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 1   | E     | 198/200 (99%) | 191 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | F     | 198/200 (99%) | 191 (96%) | 6 (3%)  | 1 (0%)   | 24          | 19  |
| 2   | M     | 229/238 (96%) | 220 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 2   | N     | 229/238 (96%) | 221 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 2   | O     | 229/238 (96%) | 218 (95%) | 11 (5%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 2   | P     | 229/238 (96%)   | 222 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 2   | Q     | 229/238 (96%)   | 223 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 2   | R     | 229/238 (96%)   | 220 (96%)  | 9 (4%)  | 0        | 100         | 100 |
| All | All   | 2562/2628 (98%) | 2470 (96%) | 91 (4%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 132 | ALA  |

### 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     | 162/163 (99%)   | 151 (93%)  | 11 (7%)  | 14          | 9  |
| 1   | B     | 162/163 (99%)   | 151 (93%)  | 11 (7%)  | 14          | 9  |
| 1   | C     | 162/163 (99%)   | 151 (93%)  | 11 (7%)  | 14          | 9  |
| 1   | D     | 162/163 (99%)   | 153 (94%)  | 9 (6%)   | 19          | 14 |
| 1   | E     | 162/163 (99%)   | 155 (96%)  | 7 (4%)   | 26          | 23 |
| 1   | F     | 162/163 (99%)   | 150 (93%)  | 12 (7%)  | 13          | 8  |
| 2   | M     | 196/202 (97%)   | 185 (94%)  | 11 (6%)  | 19          | 14 |
| 2   | N     | 196/202 (97%)   | 187 (95%)  | 9 (5%)   | 24          | 20 |
| 2   | O     | 196/202 (97%)   | 186 (95%)  | 10 (5%)  | 21          | 17 |
| 2   | P     | 196/202 (97%)   | 183 (93%)  | 13 (7%)  | 15          | 10 |
| 2   | Q     | 196/202 (97%)   | 186 (95%)  | 10 (5%)  | 21          | 17 |
| 2   | R     | 196/202 (97%)   | 186 (95%)  | 10 (5%)  | 21          | 17 |
| All | All   | 2148/2190 (98%) | 2024 (94%) | 124 (6%) | 18          | 13 |

All (124) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | LEU  |
| 1   | A     | 19  | ILE  |
| 1   | A     | 24  | GLU  |
| 1   | A     | 38  | ARG  |
| 1   | A     | 50  | LEU  |
| 1   | A     | 52  | LEU  |
| 1   | A     | 100 | ASP  |
| 1   | A     | 114 | VAL  |
| 1   | A     | 158 | LEU  |
| 1   | A     | 165 | GLN  |
| 1   | A     | 192 | GLU  |
| 2   | M     | 301 | PRO  |
| 2   | M     | 372 | LEU  |
| 2   | M     | 395 | THR  |
| 2   | M     | 411 | LYS  |
| 2   | M     | 416 | LEU  |
| 2   | M     | 428 | ARG  |
| 2   | M     | 434 | ASP  |
| 2   | M     | 440 | ARG  |
| 2   | M     | 478 | LEU  |
| 2   | M     | 497 | ASN  |
| 2   | M     | 507 | LYS  |
| 1   | B     | 4   | LEU  |
| 1   | B     | 19  | ILE  |
| 1   | B     | 24  | GLU  |
| 1   | B     | 52  | LEU  |
| 1   | B     | 78  | GLU  |
| 1   | B     | 141 | THR  |
| 1   | B     | 158 | LEU  |
| 1   | B     | 162 | GLU  |
| 1   | B     | 164 | PRO  |
| 1   | B     | 165 | GLN  |
| 1   | B     | 192 | GLU  |
| 2   | N     | 364 | LEU  |
| 2   | N     | 372 | LEU  |
| 2   | N     | 395 | THR  |
| 2   | N     | 399 | MET  |
| 2   | N     | 411 | LYS  |
| 2   | N     | 416 | LEU  |
| 2   | N     | 497 | ASN  |
| 2   | N     | 507 | LYS  |
| 2   | N     | 534 | HIS  |
| 1   | C     | 4   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 19  | ILE  |
| 1   | C     | 24  | GLU  |
| 1   | C     | 38  | ARG  |
| 1   | C     | 52  | LEU  |
| 1   | C     | 78  | GLU  |
| 1   | C     | 100 | ASP  |
| 1   | C     | 158 | LEU  |
| 1   | C     | 165 | GLN  |
| 1   | C     | 181 | THR  |
| 1   | C     | 192 | GLU  |
| 2   | O     | 364 | LEU  |
| 2   | O     | 372 | LEU  |
| 2   | O     | 393 | PRO  |
| 2   | O     | 395 | THR  |
| 2   | O     | 411 | LYS  |
| 2   | O     | 416 | LEU  |
| 2   | O     | 434 | ASP  |
| 2   | O     | 470 | ILE  |
| 2   | O     | 478 | LEU  |
| 2   | O     | 481 | GLU  |
| 1   | D     | 4   | LEU  |
| 1   | D     | 19  | ILE  |
| 1   | D     | 24  | GLU  |
| 1   | D     | 52  | LEU  |
| 1   | D     | 78  | GLU  |
| 1   | D     | 100 | ASP  |
| 1   | D     | 154 | LYS  |
| 1   | D     | 165 | GLN  |
| 1   | D     | 192 | GLU  |
| 2   | P     | 343 | ILE  |
| 2   | P     | 364 | LEU  |
| 2   | P     | 372 | LEU  |
| 2   | P     | 395 | THR  |
| 2   | P     | 411 | LYS  |
| 2   | P     | 416 | LEU  |
| 2   | P     | 428 | ARG  |
| 2   | P     | 434 | ASP  |
| 2   | P     | 440 | ARG  |
| 2   | P     | 478 | LEU  |
| 2   | P     | 497 | ASN  |
| 2   | P     | 503 | GLN  |
| 2   | P     | 534 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 4   | LEU  |
| 1   | E     | 19  | ILE  |
| 1   | E     | 24  | GLU  |
| 1   | E     | 52  | LEU  |
| 1   | E     | 100 | ASP  |
| 1   | E     | 165 | GLN  |
| 1   | E     | 192 | GLU  |
| 2   | Q     | 306 | SER  |
| 2   | Q     | 372 | LEU  |
| 2   | Q     | 395 | THR  |
| 2   | Q     | 399 | MET  |
| 2   | Q     | 416 | LEU  |
| 2   | Q     | 428 | ARG  |
| 2   | Q     | 434 | ASP  |
| 2   | Q     | 442 | ILE  |
| 2   | Q     | 497 | ASN  |
| 2   | Q     | 507 | LYS  |
| 1   | F     | 4   | LEU  |
| 1   | F     | 19  | ILE  |
| 1   | F     | 24  | GLU  |
| 1   | F     | 52  | LEU  |
| 1   | F     | 78  | GLU  |
| 1   | F     | 91  | SER  |
| 1   | F     | 100 | ASP  |
| 1   | F     | 137 | ILE  |
| 1   | F     | 154 | LYS  |
| 1   | F     | 165 | GLN  |
| 1   | F     | 181 | THR  |
| 1   | F     | 192 | GLU  |
| 2   | R     | 372 | LEU  |
| 2   | R     | 395 | THR  |
| 2   | R     | 411 | LYS  |
| 2   | R     | 416 | LEU  |
| 2   | R     | 428 | ARG  |
| 2   | R     | 434 | ASP  |
| 2   | R     | 442 | ILE  |
| 2   | R     | 478 | LEU  |
| 2   | R     | 497 | ASN  |
| 2   | R     | 503 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 59  | ASN  |
| 1   | A     | 127 | ASN  |
| 1   | A     | 136 | ASN  |
| 1   | A     | 165 | GLN  |
| 2   | M     | 361 | HIS  |
| 2   | M     | 412 | ASN  |
| 2   | M     | 497 | ASN  |
| 2   | M     | 503 | GLN  |
| 2   | M     | 530 | GLN  |
| 1   | B     | 159 | ASN  |
| 1   | B     | 165 | GLN  |
| 2   | N     | 314 | ASN  |
| 2   | N     | 334 | GLN  |
| 2   | N     | 359 | HIS  |
| 2   | N     | 361 | HIS  |
| 2   | N     | 412 | ASN  |
| 2   | N     | 497 | ASN  |
| 2   | N     | 503 | GLN  |
| 1   | C     | 11  | GLN  |
| 1   | C     | 163 | GLN  |
| 1   | C     | 165 | GLN  |
| 2   | O     | 361 | HIS  |
| 2   | O     | 412 | ASN  |
| 2   | O     | 497 | ASN  |
| 2   | O     | 503 | GLN  |
| 2   | O     | 530 | GLN  |
| 1   | D     | 54  | GLN  |
| 1   | D     | 140 | HIS  |
| 1   | D     | 163 | GLN  |
| 1   | D     | 165 | GLN  |
| 2   | P     | 359 | HIS  |
| 2   | P     | 361 | HIS  |
| 2   | P     | 394 | ASN  |
| 2   | P     | 497 | ASN  |
| 2   | P     | 514 | ASN  |
| 1   | E     | 11  | GLN  |
| 1   | E     | 163 | GLN  |
| 1   | E     | 165 | GLN  |
| 2   | Q     | 361 | HIS  |
| 2   | Q     | 412 | ASN  |
| 2   | Q     | 422 | ASN  |
| 2   | Q     | 497 | ASN  |
| 2   | Q     | 503 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 140 | HIS  |
| 1   | F     | 163 | GLN  |
| 1   | F     | 165 | GLN  |
| 2   | R     | 361 | HIS  |
| 2   | R     | 412 | ASN  |
| 2   | R     | 422 | ASN  |
| 2   | R     | 497 | ASN  |
| 2   | R     | 511 | 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 [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | BME  | N     | 601 | 2    | 3,3,3        | 0.24 | 0           | 2,2,2       | 0.43 | 0           |
| 4   | BME  | O     | 601 | 2    | 3,3,3        | 0.46 | 0           | 2,2,2       | 0.74 | 0           |
| 5   | NNO  | Q     | 550 | 3    | 11,11,11     | 2.11 | 4 (36%)     | 11,15,15    | 1.31 | 2 (18%)     |
| 5   | NNO  | O     | 550 | 3    | 11,11,11     | 2.15 | 5 (45%)     | 11,15,15    | 1.61 | 2 (18%)     |
| 4   | BME  | R     | 601 | 2    | 3,3,3        | 0.48 | 0           | 2,2,2       | 0.35 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | NNO  | P     | 550 | 3    | 11,11,11     | 2.22 | 3 (27%)  | 11,15,15    | 1.51 | 2 (18%)  |
| 4   | BME  | P     | 601 | 2    | 3,3,3        | 0.58 | 0        | 2,2,2       | 0.83 | 0        |
| 4   | BME  | M     | 601 | 2    | 3,3,3        | 0.43 | 0        | 2,2,2       | 0.61 | 0        |
| 5   | NNO  | M     | 550 | 3    | 11,11,11     | 2.32 | 5 (45%)  | 11,15,15    | 1.53 | 1 (9%)   |
| 5   | NNO  | N     | 550 | 3    | 11,11,11     | 2.11 | 5 (45%)  | 11,15,15    | 1.39 | 2 (18%)  |
| 5   | NNO  | R     | 550 | 3    | 11,11,11     | 2.01 | 3 (27%)  | 11,15,15    | 1.46 | 2 (18%)  |
| 4   | BME  | Q     | 601 | 2    | 3,3,3        | 0.75 | 0        | 2,2,2       | 0.81 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 4   | BME  | N     | 601 | 2    | -       | 0/1/1/1  | -       |
| 4   | BME  | O     | 601 | 2    | -       | 0/1/1/1  | -       |
| 5   | NNO  | Q     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 5   | NNO  | O     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 4   | BME  | R     | 601 | 2    | -       | 0/1/1/1  | -       |
| 5   | NNO  | P     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 4   | BME  | P     | 601 | 2    | -       | 0/1/1/1  | -       |
| 4   | BME  | M     | 601 | 2    | -       | 0/1/1/1  | -       |
| 5   | NNO  | M     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 5   | NNO  | N     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 5   | NNO  | R     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 4   | BME  | Q     | 601 | 2    | -       | 0/1/1/1  | -       |

All (25) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | M     | 550 | NNO  | O3-N1 | -5.89 | 1.25        | 1.37     |
| 5   | P     | 550 | NNO  | O3-N1 | -5.68 | 1.26        | 1.37     |
| 5   | O     | 550 | NNO  | O3-N1 | -5.26 | 1.26        | 1.37     |
| 5   | Q     | 550 | NNO  | O3-N1 | -5.07 | 1.27        | 1.37     |
| 5   | R     | 550 | NNO  | O3-N1 | -5.05 | 1.27        | 1.37     |
| 5   | N     | 550 | NNO  | O3-N1 | -5.03 | 1.27        | 1.37     |
| 5   | P     | 550 | NNO  | C3-C7 | 3.23  | 1.56        | 1.49     |
| 5   | Q     | 550 | NNO  | C2-C3 | 2.93  | 1.43        | 1.39     |
| 5   | N     | 550 | NNO  | C3-C7 | 2.46  | 1.54        | 1.49     |
| 5   | M     | 550 | NNO  | C2-C3 | 2.45  | 1.42        | 1.39     |
| 5   | M     | 550 | NNO  | O2-C7 | -2.38 | 1.23        | 1.30     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | M     | 550 | NNO  | C3-C7 | 2.37  | 1.54        | 1.49     |
| 5   | O     | 550 | NNO  | C2-C3 | 2.37  | 1.42        | 1.39     |
| 5   | P     | 550 | NNO  | O2-C7 | -2.35 | 1.23        | 1.30     |
| 5   | O     | 550 | NNO  | C3-C7 | 2.33  | 1.54        | 1.49     |
| 5   | Q     | 550 | NNO  | O2-C7 | -2.20 | 1.24        | 1.30     |
| 5   | N     | 550 | NNO  | O2-C7 | -2.18 | 1.24        | 1.30     |
| 5   | O     | 550 | NNO  | O2-C7 | -2.18 | 1.24        | 1.30     |
| 5   | R     | 550 | NNO  | C3-C7 | 2.13  | 1.54        | 1.49     |
| 5   | R     | 550 | NNO  | O2-C7 | -2.11 | 1.24        | 1.30     |
| 5   | N     | 550 | NNO  | C2-C3 | 2.11  | 1.42        | 1.39     |
| 5   | Q     | 550 | NNO  | C3-C7 | 2.08  | 1.53        | 1.49     |
| 5   | M     | 550 | NNO  | C2-N1 | -2.07 | 1.31        | 1.35     |
| 5   | O     | 550 | NNO  | C2-N1 | -2.02 | 1.31        | 1.35     |
| 5   | N     | 550 | NNO  | C2-N1 | -2.01 | 1.31        | 1.35     |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | O     | 550 | NNO  | O2-C7-C3 | 3.10  | 122.79      | 114.84   |
| 5   | M     | 550 | NNO  | O2-C7-C3 | 2.92  | 122.34      | 114.84   |
| 5   | P     | 550 | NNO  | O2-C7-C3 | 2.75  | 121.88      | 114.84   |
| 5   | R     | 550 | NNO  | O2-C7-O1 | -2.72 | 117.50      | 123.35   |
| 5   | O     | 550 | NNO  | O2-C7-O1 | -2.71 | 117.53      | 123.35   |
| 5   | P     | 550 | NNO  | O2-C7-O1 | -2.69 | 117.57      | 123.35   |
| 5   | N     | 550 | NNO  | O2-C7-C3 | 2.54  | 121.34      | 114.84   |
| 5   | Q     | 550 | NNO  | O2-C7-O1 | -2.36 | 118.29      | 123.35   |
| 5   | R     | 550 | NNO  | O2-C7-C3 | 2.31  | 120.77      | 114.84   |
| 5   | Q     | 550 | NNO  | O2-C7-C3 | 2.31  | 120.77      | 114.84   |
| 5   | N     | 550 | NNO  | O2-C7-O1 | -2.24 | 118.54      | 123.35   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | N     | 601 | BME  | 2       | 0            |
| 4   | O     | 601 | BME  | 2       | 0            |
| 4   | Q     | 601 | BME  | 2       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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.