



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:08 AM UTC

PDB ID : 3PCJ / pdb\_00003pcj  
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-  
PLEXED WITH 2-HYDROXYISONICOTINIC 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                                                             |

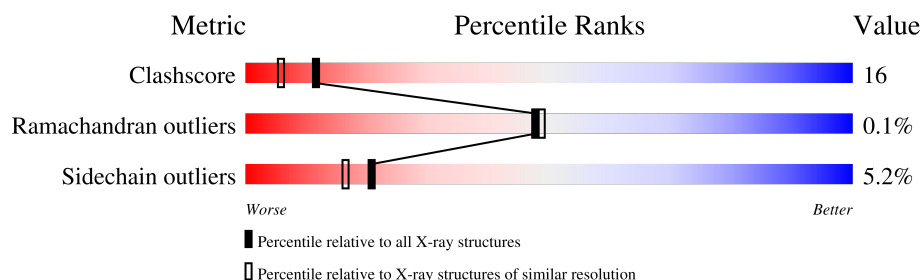
# 1 Overall quality at a glance

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    |                  |
| 1   | B     | 200    |                  |
| 1   | C     | 200    |                  |
| 1   | D     | 200    |                  |
| 1   | E     | 200    |                  |
| 1   | F     | 200    |                  |
| 2   | M     | 238    |                  |
| 2   | N     | 238    |                  |

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| Mol | Chain | Length | Quality of chain                                     |
|-----|-------|--------|------------------------------------------------------|
| 2   | O     | 238    | <div><div></div><div>59%31%8%</div><div></div></div> |
| 2   | P     | 238    | <div><div></div><div>62%29%7%</div><div></div></div> |
| 2   | Q     | 238    | <div><div></div><div>63%29%6%</div><div></div></div> |
| 2   | R     | 238    | <div><div></div><div>56%32%9%</div><div></div></div> |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21978 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 |         |         |       |

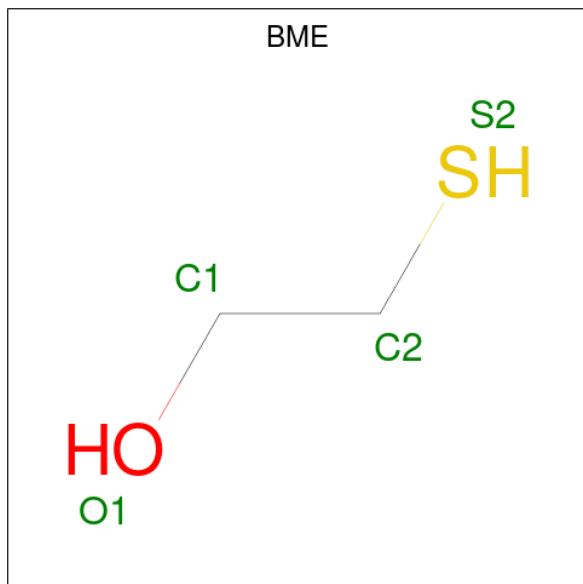
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

| 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).

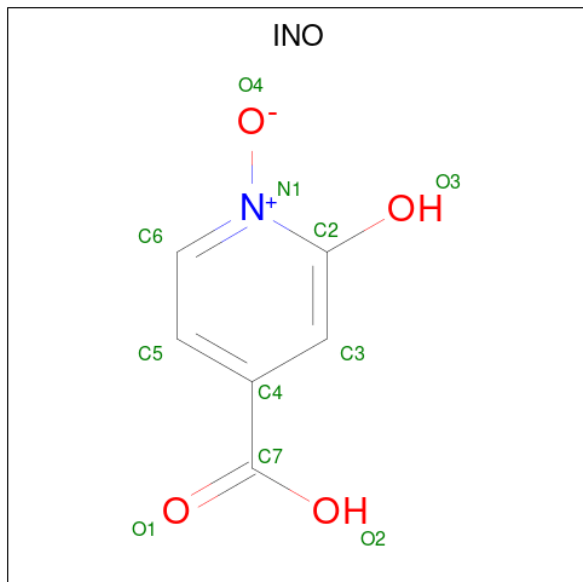
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | M     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 3   | N     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 3   | O     | 1        | Total Fe<br>1 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:  $C_2H_6OS$ ).



| 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 2-HYDROXYISONICOTINIC ACID N-OXIDE (CCD ID: INO) (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     | 79       | Total | O   | 0       | 0       |
|     |       |          | 79    | 79  |         |         |
| 6   | M     | 155      | Total | O   | 0       | 0       |
|     |       |          | 155   | 155 |         |         |
| 6   | B     | 78       | Total | O   | 0       | 0       |
|     |       |          | 78    | 78  |         |         |
| 6   | N     | 163      | Total | O   | 0       | 0       |
|     |       |          | 163   | 163 |         |         |

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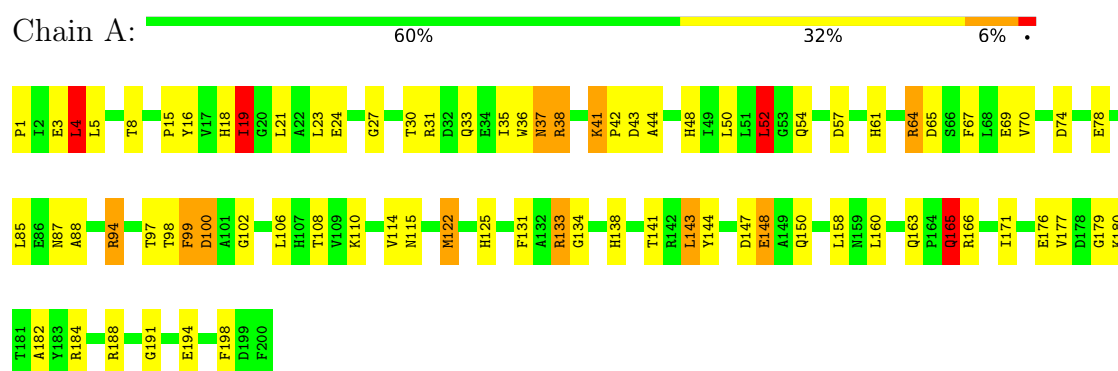
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 6   | C     | 76       | Total<br>76  | O<br>76  | 0       | 0       |
| 6   | O     | 158      | Total<br>158 | O<br>158 | 0       | 0       |
| 6   | D     | 79       | Total<br>79  | O<br>79  | 0       | 0       |
| 6   | P     | 149      | Total<br>149 | O<br>149 | 0       | 0       |
| 6   | E     | 81       | Total<br>81  | O<br>81  | 0       | 0       |
| 6   | Q     | 160      | Total<br>160 | O<br>160 | 0       | 0       |
| 6   | F     | 75       | Total<br>75  | O<br>75  | 0       | 0       |
| 6   | R     | 163      | Total<br>163 | O<br>163 | 0       | 0       |

### 3 Residue-property plots

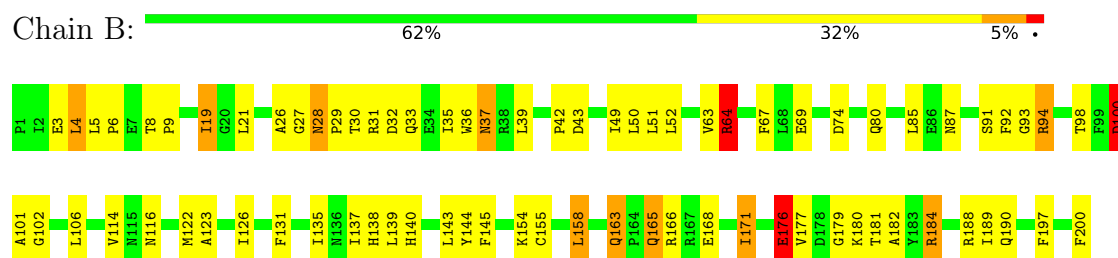
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

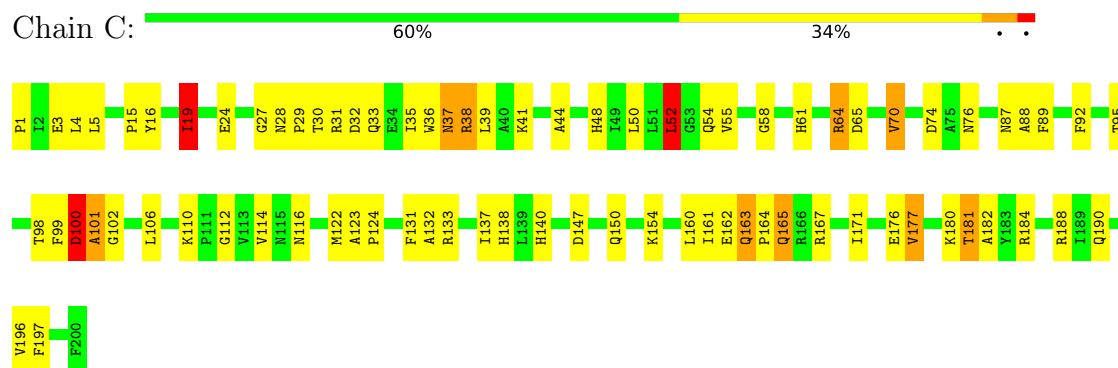
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



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

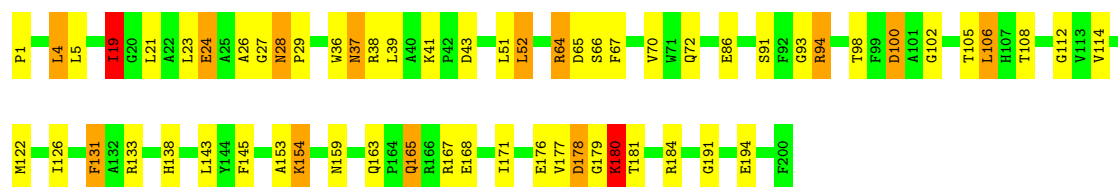


#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



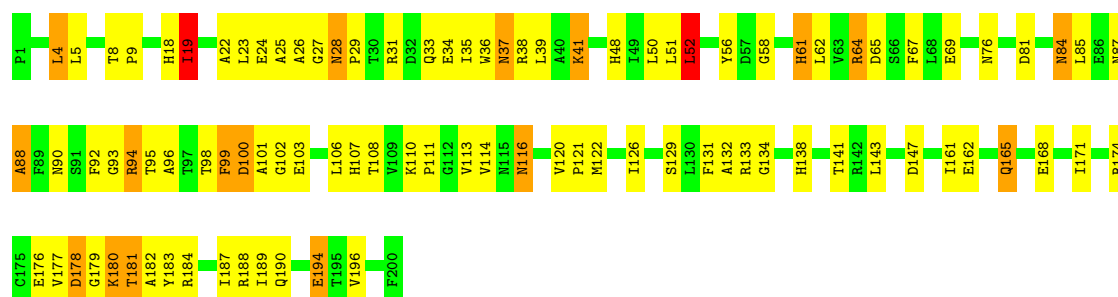
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain D:  70% 23% 6% •



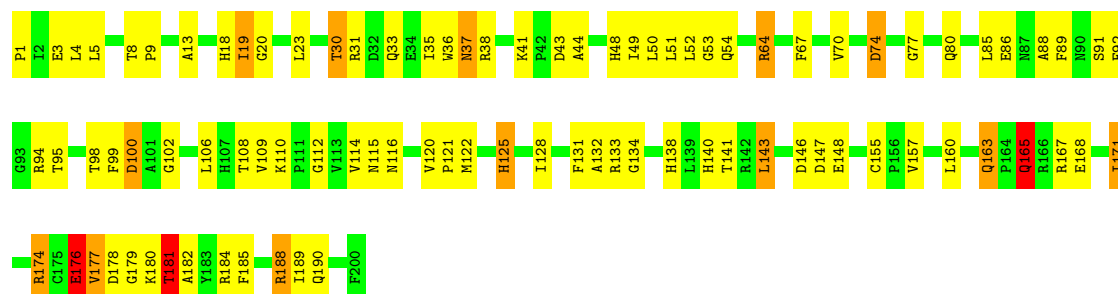
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain E:  52% 38% 8% •



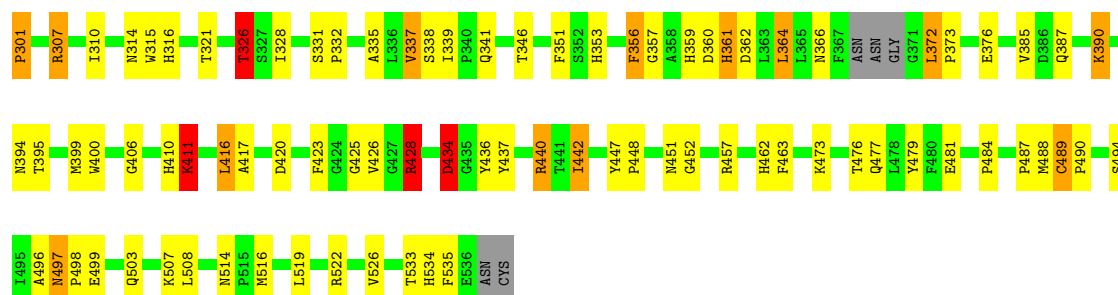
• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain F:  54% 38% 6% •



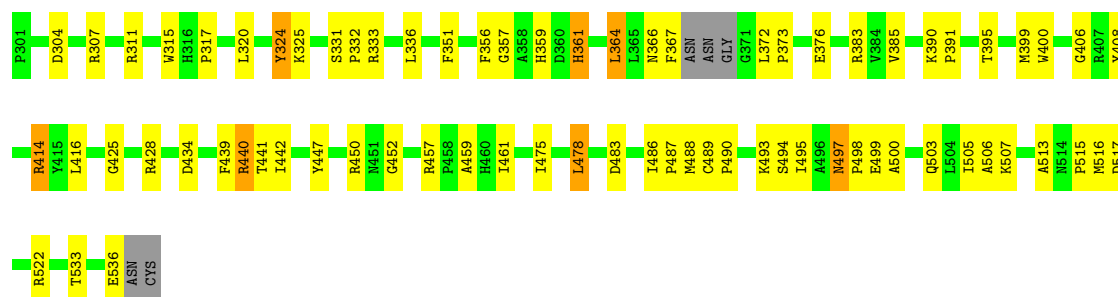
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain M:  62% 29% 5% • •



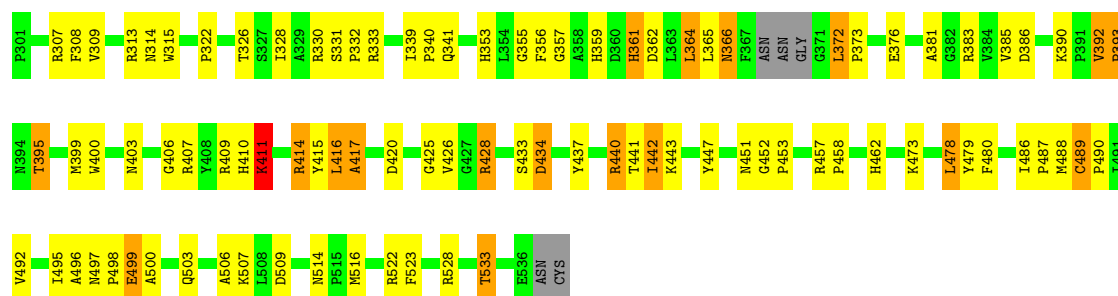
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain N:  67% 28% . .



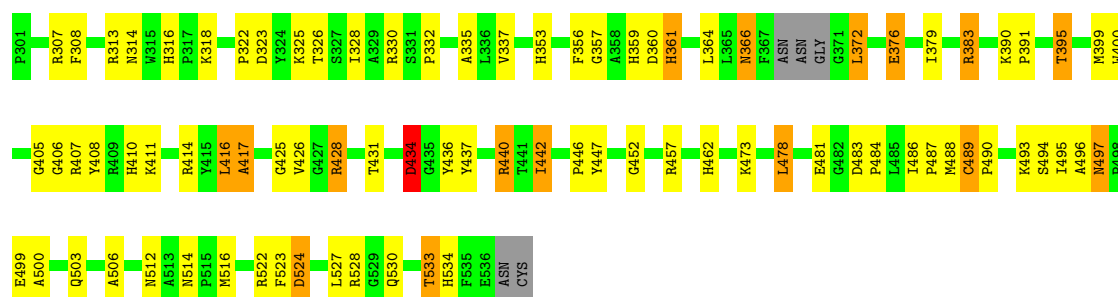
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain O:  59% 31% 8% .



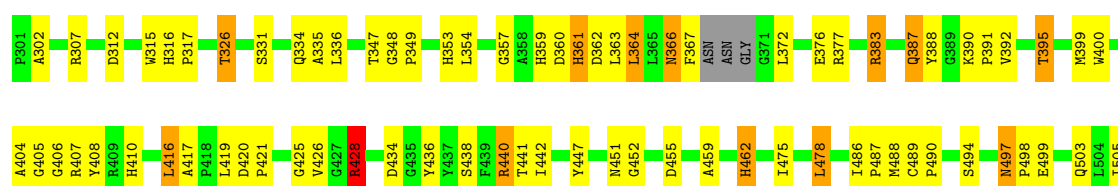
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P:  62% 29% 7% .



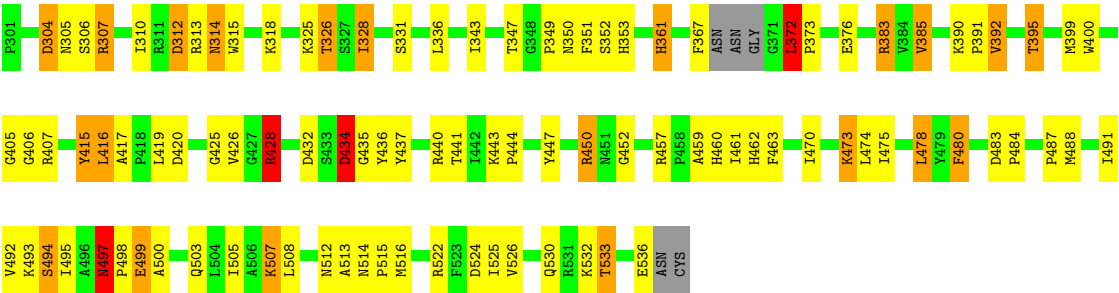
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q:  63% 29% 6% .





● 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, $\alpha$ , $\beta$ , $\gamma$ | 196.20 Å   127.10 Å   133.70 Å<br>90.00°   97.70°   90.00° | Depositor |
| Resolution (Å)                                           | 6.00 – 2.13                                                | Depositor |
| % Data completeness<br>(in resolution range)             | 96.0 (6.00-2.13)                                           | Depositor |
| $R_{merge}$                                              | (Not available)                                            | Depositor |
| $R_{sym}$                                                | 0.07                                                       | 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                                    | 21978                                                      | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 26.0                                                       | 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: INO, BME, FE

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     | 1.27         | 4/1611 (0.2%)   | 1.91        | 37/2195 (1.7%)   |
| 1   | B     | 1.25         | 2/1611 (0.1%)   | 1.89        | 36/2195 (1.6%)   |
| 1   | C     | 1.28         | 1/1611 (0.1%)   | 1.86        | 30/2195 (1.4%)   |
| 1   | D     | 1.28         | 1/1611 (0.1%)   | 1.77        | 27/2195 (1.2%)   |
| 1   | E     | 1.32         | 3/1611 (0.2%)   | 1.87        | 32/2195 (1.5%)   |
| 1   | F     | 1.39         | 6/1611 (0.4%)   | 1.91        | 35/2195 (1.6%)   |
| 2   | M     | 1.33         | 1/1895 (0.1%)   | 1.93        | 37/2580 (1.4%)   |
| 2   | N     | 1.34         | 5/1895 (0.3%)   | 1.85        | 28/2580 (1.1%)   |
| 2   | O     | 1.37         | 3/1895 (0.2%)   | 1.92        | 54/2580 (2.1%)   |
| 2   | P     | 1.35         | 4/1895 (0.2%)   | 1.87        | 40/2580 (1.6%)   |
| 2   | Q     | 1.39         | 4/1895 (0.2%)   | 1.83        | 26/2580 (1.0%)   |
| 2   | R     | 1.40         | 4/1895 (0.2%)   | 1.92        | 45/2580 (1.7%)   |
| All | All   | 1.33         | 38/21036 (0.2%) | 1.88        | 427/28650 (1.5%) |

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   | B     | 0                   | 1                   |
| 2   | R     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (38) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | O     | 451 | ASN  | CA-C  | 10.39 | 1.57        | 1.52     |
| 1   | C     | 100 | ASP  | N-CA  | 7.67  | 1.51        | 1.46     |
| 1   | A     | 94  | ARG  | CD-NE | -7.65 | 1.35        | 1.46     |
| 2   | N     | 441 | THR  | CA-CB | 7.15  | 1.62        | 1.54     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | F     | 128 | ILE  | CA-CB | 6.17  | 1.63        | 1.54     |
| 2   | Q     | 441 | THR  | CA-CB | 6.13  | 1.61        | 1.53     |
| 2   | N     | 452 | GLY  | N-CA  | 6.07  | 1.52        | 1.44     |
| 1   | D     | 108 | THR  | CA-CB | 6.02  | 1.62        | 1.54     |
| 1   | F     | 133 | ARG  | CD-NE | -5.92 | 1.38        | 1.46     |
| 2   | P     | 379 | ILE  | C-O   | 5.88  | 1.30        | 1.24     |
| 2   | O     | 506 | ALA  | N-CA  | 5.87  | 1.53        | 1.46     |
| 2   | Q     | 462 | HIS  | N-CA  | 5.86  | 1.53        | 1.46     |
| 1   | F     | 13  | ALA  | C-O   | 5.81  | 1.31        | 1.24     |
| 2   | M     | 321 | THR  | N-CA  | 5.76  | 1.52        | 1.46     |
| 2   | O     | 441 | THR  | CA-CB | 5.68  | 1.61        | 1.54     |
| 1   | E     | 108 | THR  | CA-CB | 5.61  | 1.61        | 1.53     |
| 1   | A     | 108 | THR  | CA-CB | 5.61  | 1.61        | 1.53     |
| 1   | F     | 140 | HIS  | CA-CB | 5.59  | 1.62        | 1.53     |
| 1   | A     | 8   | THR  | N-CA  | 5.53  | 1.52        | 1.45     |
| 2   | R     | 525 | ILE  | CA-CB | 5.41  | 1.61        | 1.54     |
| 2   | R     | 483 | ASP  | N-CA  | 5.38  | 1.54        | 1.46     |
| 2   | P     | 452 | GLY  | N-CA  | 5.33  | 1.52        | 1.44     |
| 2   | Q     | 367 | PHE  | C-O   | 5.25  | 1.34        | 1.23     |
| 1   | F     | 171 | ILE  | CA-CB | 5.24  | 1.60        | 1.54     |
| 2   | R     | 441 | THR  | CA-CB | 5.24  | 1.61        | 1.54     |
| 2   | P     | 332 | PRO  | C-O   | 5.23  | 1.29        | 1.23     |
| 1   | B     | 63  | VAL  | N-CA  | 5.22  | 1.52        | 1.46     |
| 1   | F     | 108 | THR  | CA-CB | 5.15  | 1.60        | 1.53     |
| 2   | N     | 506 | ALA  | C-O   | 5.14  | 1.30        | 1.23     |
| 2   | Q     | 428 | ARG  | CD-NE | -5.12 | 1.39        | 1.46     |
| 1   | B     | 94  | ARG  | CD-NE | -5.09 | 1.39        | 1.46     |
| 1   | A     | 4   | LEU  | N-CA  | 5.07  | 1.52        | 1.45     |
| 2   | N     | 317 | PRO  | C-O   | 5.06  | 1.29        | 1.23     |
| 1   | E     | 187 | ILE  | C-N   | -5.05 | 1.26        | 1.33     |
| 2   | P     | 478 | LEU  | N-CA  | 5.04  | 1.52        | 1.46     |
| 2   | N     | 320 | LEU  | C-N   | -5.04 | 1.27        | 1.33     |
| 2   | R     | 417 | ALA  | N-CA  | 5.02  | 1.52        | 1.45     |
| 1   | E     | 113 | VAL  | CA-CB | 5.01  | 1.59        | 1.54     |

All (427) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | F     | 133 | ARG  | CD-NE-CZ | 17.57  | 149.00      | 124.40   |
| 1   | A     | 94  | ARG  | CD-NE-CZ | 14.74  | 145.04      | 124.40   |
| 2   | O     | 353 | HIS  | CA-CB-CG | -12.42 | 101.38      | 113.80   |
| 1   | A     | 87  | ASN  | CA-CB-CG | 12.24  | 124.84      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 2   | N     | 440 | ARG  | NE-CZ-NH2  | -12.08 | 108.33      | 119.20   |
| 2   | R     | 440 | ARG  | NE-CZ-NH2  | -11.39 | 108.95      | 119.20   |
| 2   | M     | 440 | ARG  | NE-CZ-NH2  | -11.08 | 109.22      | 119.20   |
| 2   | O     | 452 | GLY  | N-CA-C     | -10.56 | 99.45       | 112.23   |
| 2   | R     | 361 | HIS  | CA-CB-CG   | -10.55 | 103.25      | 113.80   |
| 2   | R     | 434 | ASP  | CA-CB-CG   | -10.23 | 102.37      | 112.60   |
| 2   | P     | 440 | ARG  | NE-CZ-NH2  | -10.22 | 110.00      | 119.20   |
| 2   | M     | 457 | ARG  | CD-NE-CZ   | 9.72   | 138.01      | 124.40   |
| 2   | R     | 353 | HIS  | CA-CB-CG   | -9.70  | 104.10      | 113.80   |
| 2   | O     | 440 | ARG  | NE-CZ-NH2  | -9.66  | 110.50      | 119.20   |
| 1   | D     | 37  | ASN  | N-CA-C     | 9.57   | 123.65      | 112.93   |
| 1   | B     | 176 | GLU  | CB-CG-CD   | 9.48   | 128.71      | 112.60   |
| 2   | N     | 452 | GLY  | N-CA-C     | -9.25  | 101.04      | 112.23   |
| 1   | B     | 64  | ARG  | CD-NE-CZ   | -9.24  | 111.46      | 124.40   |
| 2   | O     | 434 | ASP  | CA-CB-CG   | -9.18  | 103.42      | 112.60   |
| 2   | O     | 451 | ASN  | O-C-N      | 9.07   | 128.88      | 120.71   |
| 2   | Q     | 452 | GLY  | N-CA-C     | -8.97  | 101.07      | 112.10   |
| 2   | O     | 451 | ASN  | CA-C-O     | -8.95  | 114.09      | 119.55   |
| 1   | A     | 37  | ASN  | N-CA-C     | 8.93   | 123.47      | 113.21   |
| 1   | C     | 37  | ASN  | N-CA-C     | 8.88   | 122.88      | 112.93   |
| 1   | F     | 64  | ARG  | CD-NE-CZ   | -8.87  | 111.98      | 124.40   |
| 2   | M     | 494 | SER  | N-CA-C     | -8.87  | 101.54      | 111.82   |
| 1   | A     | 94  | ARG  | CG-CD-NE   | 8.82   | 131.41      | 112.00   |
| 1   | B     | 37  | ASN  | N-CA-C     | 8.79   | 122.77      | 112.93   |
| 1   | D     | 19  | ILE  | CB-CA-C    | 8.49   | 123.16      | 112.04   |
| 2   | Q     | 440 | ARG  | NE-CZ-NH2  | -8.48  | 111.57      | 119.20   |
| 1   | A     | 94  | ARG  | CB-CG-CD   | 8.36   | 130.54      | 111.30   |
| 2   | N     | 414 | ARG  | CD-NE-CZ   | -8.34  | 112.72      | 124.40   |
| 2   | N     | 522 | ARG  | CD-NE-CZ   | 8.30   | 136.03      | 124.40   |
| 1   | A     | 166 | ARG  | CD-NE-CZ   | 8.28   | 135.99      | 124.40   |
| 1   | A     | 3   | GLU  | CB-CG-CD   | 8.21   | 126.56      | 112.60   |
| 2   | O     | 457 | ARG  | CD-NE-CZ   | 8.10   | 135.74      | 124.40   |
| 1   | B     | 64  | ARG  | NE-CZ-NH1  | -8.09  | 113.41      | 121.50   |
| 1   | D     | 167 | ARG  | CD-NE-CZ   | 8.04   | 135.66      | 124.40   |
| 2   | Q     | 383 | ARG  | CD-NE-CZ   | -8.02  | 113.18      | 124.40   |
| 2   | N     | 434 | ASP  | CA-CB-CG   | -7.96  | 104.64      | 112.60   |
| 1   | E     | 107 | HIS  | CA-CB-CG   | -7.85  | 105.95      | 113.80   |
| 1   | C     | 38  | ARG  | CD-NE-CZ   | -7.82  | 113.45      | 124.40   |
| 2   | N     | 383 | ARG  | CD-NE-CZ   | -7.82  | 113.46      | 124.40   |
| 1   | A     | 64  | ARG  | CD-NE-CZ   | -7.79  | 113.49      | 124.40   |
| 2   | M     | 477 | GLN  | OE1-CD-NE2 | -7.74  | 114.86      | 122.60   |
| 2   | P     | 514 | ASN  | CA-CB-CG   | 7.69   | 120.29      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 64  | ARG  | NE-CZ-NH1  | -7.64 | 113.86      | 121.50   |
| 1   | F     | 64  | ARG  | NE-CZ-NH1  | -7.62 | 113.88      | 121.50   |
| 2   | R     | 312 | ASP  | CA-CB-CG   | -7.62 | 104.98      | 112.60   |
| 2   | M     | 361 | HIS  | CA-CB-CG   | -7.53 | 106.27      | 113.80   |
| 1   | F     | 37  | ASN  | N-CA-C     | 7.53  | 122.11      | 113.15   |
| 1   | F     | 176 | GLU  | CB-CG-CD   | 7.47  | 125.30      | 112.60   |
| 1   | B     | 184 | ARG  | NE-CZ-NH2  | -7.46 | 112.48      | 119.20   |
| 1   | A     | 23  | LEU  | CB-CA-C    | 7.45  | 123.21      | 110.84   |
| 2   | Q     | 348 | GLY  | O-C-N      | 7.41  | 129.18      | 121.77   |
| 2   | P     | 533 | THR  | CA-CB-OG1  | -7.37 | 98.55       | 109.60   |
| 1   | E     | 64  | ARG  | CD-NE-CZ   | -7.36 | 114.09      | 124.40   |
| 1   | E     | 37  | ASN  | N-CA-C     | 7.36  | 121.90      | 113.15   |
| 2   | Q     | 361 | HIS  | CA-CB-CG   | -7.35 | 106.45      | 113.80   |
| 2   | M     | 434 | ASP  | CA-CB-CG   | -7.28 | 105.32      | 112.60   |
| 2   | R     | 336 | LEU  | CA-C-O     | -7.16 | 113.57      | 121.87   |
| 2   | Q     | 434 | ASP  | CA-CB-CG   | -7.12 | 105.48      | 112.60   |
| 2   | P     | 314 | ASN  | N-CA-C     | -7.12 | 104.75      | 113.50   |
| 1   | B     | 94  | ARG  | CB-CG-CD   | 7.11  | 127.64      | 111.30   |
| 1   | E     | 64  | ARG  | NE-CZ-NH1  | -7.10 | 114.40      | 121.50   |
| 1   | E     | 5   | LEU  | N-CA-C     | -7.10 | 100.29      | 110.08   |
| 2   | R     | 392 | VAL  | O-C-N      | 7.09  | 127.77      | 120.96   |
| 1   | B     | 94  | ARG  | CG-CD-NE   | 7.05  | 127.51      | 112.00   |
| 2   | P     | 372 | LEU  | CB-CA-C    | 7.05  | 118.48      | 108.68   |
| 2   | O     | 341 | GLN  | OE1-CD-NE2 | -7.03 | 115.57      | 122.60   |
| 2   | N     | 361 | HIS  | CA-CB-CG   | -7.02 | 106.78      | 113.80   |
| 1   | E     | 38  | ARG  | CD-NE-CZ   | -7.01 | 114.59      | 124.40   |
| 1   | A     | 150 | GLN  | OE1-CD-NE2 | -6.99 | 115.61      | 122.60   |
| 1   | E     | 189 | ILE  | O-C-N      | 6.99  | 128.65      | 121.87   |
| 1   | C     | 52  | LEU  | CB-CA-C    | 6.92  | 125.33      | 110.45   |
| 2   | M     | 516 | MET  | CA-C-O     | -6.90 | 112.17      | 120.32   |
| 1   | A     | 177 | VAL  | O-C-N      | 6.90  | 130.14      | 123.03   |
| 1   | A     | 166 | ARG  | NE-CZ-NH1  | 6.90  | 128.40      | 121.50   |
| 1   | F     | 167 | ARG  | CD-NE-CZ   | -6.88 | 114.76      | 124.40   |
| 1   | C     | 150 | GLN  | N-CA-CB    | 6.88  | 119.96      | 109.91   |
| 2   | M     | 353 | HIS  | CA-CB-CG   | -6.78 | 107.02      | 113.80   |
| 1   | F     | 163 | GLN  | CA-C-O     | 6.76  | 123.68      | 119.29   |
| 2   | N     | 475 | ILE  | N-CA-CB    | 6.74  | 120.71      | 111.41   |
| 2   | R     | 514 | ASN  | CA-CB-CG   | 6.72  | 119.32      | 112.60   |
| 1   | F     | 5   | LEU  | N-CA-C     | -6.70 | 100.83      | 110.08   |
| 2   | R     | 499 | GLU  | N-CA-CB    | 6.70  | 120.67      | 110.28   |
| 1   | D     | 94  | ARG  | NE-CZ-NH2  | -6.70 | 113.17      | 119.20   |
| 1   | E     | 19  | ILE  | CB-CA-C    | 6.70  | 120.82      | 112.04   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 30  | THR  | CA-CB-OG1  | -6.67 | 99.60       | 109.60   |
| 2   | P     | 434 | ASP  | CA-CB-CG   | -6.65 | 105.95      | 112.60   |
| 2   | P     | 323 | ASP  | CA-CB-CG   | -6.64 | 105.96      | 112.60   |
| 2   | R     | 457 | ARG  | CA-CB-CG   | 6.61  | 127.31      | 114.10   |
| 1   | D     | 86  | GLU  | CB-CG-CD   | 6.58  | 123.80      | 112.60   |
| 2   | Q     | 514 | ASN  | O-C-N      | 6.58  | 127.38      | 121.19   |
| 1   | B     | 171 | ILE  | N-CA-C     | 6.58  | 117.32      | 107.51   |
| 1   | E     | 90  | ASN  | OD1-CG-ND2 | -6.58 | 116.02      | 122.60   |
| 2   | R     | 450 | ARG  | CD-NE-CZ   | -6.55 | 115.22      | 124.40   |
| 2   | M     | 514 | ASN  | O-C-N      | 6.55  | 128.59      | 121.12   |
| 1   | A     | 115 | ASN  | CA-CB-CG   | 6.54  | 119.14      | 112.60   |
| 1   | F     | 86  | GLU  | CB-CG-CD   | 6.54  | 123.72      | 112.60   |
| 2   | P     | 361 | HIS  | CA-CB-CG   | -6.54 | 107.26      | 113.80   |
| 1   | C     | 87  | ASN  | CA-CB-CG   | 6.53  | 119.13      | 112.60   |
| 2   | O     | 496 | ALA  | CA-C-O     | -6.52 | 113.64      | 120.55   |
| 2   | M     | 479 | TYR  | CA-C-O     | -6.52 | 113.83      | 121.46   |
| 2   | P     | 353 | HIS  | CA-CB-CG   | -6.51 | 107.29      | 113.80   |
| 1   | D     | 64  | ARG  | NE-CZ-NH1  | -6.50 | 115.00      | 121.50   |
| 2   | R     | 494 | SER  | N-CA-C     | -6.50 | 104.61      | 112.54   |
| 2   | Q     | 377 | ARG  | NE-CZ-NH1  | -6.50 | 115.00      | 121.50   |
| 2   | N     | 336 | LEU  | CA-C-O     | -6.48 | 114.49      | 121.56   |
| 2   | Q     | 533 | THR  | CA-CB-OG1  | -6.47 | 99.89       | 109.60   |
| 1   | F     | 171 | ILE  | N-CA-CB    | -6.46 | 103.64      | 111.00   |
| 2   | O     | 322 | PRO  | CB-CA-C    | 6.46  | 122.22      | 111.56   |
| 2   | M     | 417 | ALA  | N-CA-C     | -6.46 | 101.93      | 109.93   |
| 1   | F     | 133 | ARG  | NE-CZ-NH1  | 6.45  | 127.95      | 121.50   |
| 2   | P     | 512 | ASN  | CA-CB-CG   | -6.45 | 106.16      | 112.60   |
| 1   | E     | 90  | ASN  | CA-CB-CG   | 6.45  | 119.05      | 112.60   |
| 1   | E     | 48  | HIS  | CA-CB-CG   | -6.43 | 107.37      | 113.80   |
| 2   | R     | 336 | LEU  | N-CA-C     | -6.43 | 102.05      | 110.53   |
| 2   | Q     | 535 | PHE  | CA-CB-CG   | 6.42  | 120.22      | 113.80   |
| 2   | N     | 325 | LYS  | CA-C-N     | 6.42  | 129.18      | 120.38   |
| 2   | N     | 325 | LYS  | C-N-CA     | 6.42  | 129.18      | 120.38   |
| 2   | N     | 385 | VAL  | CA-C-O     | -6.41 | 115.13      | 121.67   |
| 2   | M     | 496 | ALA  | N-CA-C     | 6.40  | 117.92      | 111.07   |
| 2   | R     | 492 | VAL  | N-CA-C     | -6.39 | 104.10      | 110.30   |
| 1   | E     | 88  | ALA  | N-CA-C     | -6.37 | 104.20      | 112.23   |
| 2   | R     | 307 | ARG  | N-CA-C     | -6.35 | 99.47       | 109.50   |
| 1   | D     | 38  | ARG  | CD-NE-CZ   | -6.33 | 115.54      | 124.40   |
| 2   | N     | 439 | PHE  | O-C-N      | 6.32  | 130.82      | 123.17   |
| 2   | P     | 330 | ARG  | CD-NE-CZ   | -6.31 | 115.56      | 124.40   |
| 1   | F     | 140 | HIS  | CB-CA-C    | -6.27 | 98.95       | 109.48   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | O     | 339 | ILE  | O-C-N     | 6.25  | 128.23      | 121.10   |
| 1   | B     | 200 | PHE  | CA-CB-CG  | 6.25  | 120.05      | 113.80   |
| 2   | N     | 517 | ASP  | CA-CB-CG  | 6.25  | 118.85      | 112.60   |
| 2   | M     | 394 | ASN  | CA-C-O    | -6.24 | 114.60      | 121.84   |
| 2   | N     | 367 | PHE  | CA-C-O    | -6.23 | 110.22      | 120.80   |
| 2   | O     | 361 | HIS  | CA-CB-CG  | -6.21 | 107.59      | 113.80   |
| 2   | O     | 308 | PHE  | CA-CB-CG  | -6.20 | 107.60      | 113.80   |
| 1   | D     | 64  | ARG  | CD-NE-CZ  | -6.19 | 115.73      | 124.40   |
| 1   | B     | 189 | ILE  | O-C-N     | 6.17  | 128.18      | 121.83   |
| 2   | M     | 326 | THR  | CA-CB-OG1 | -6.16 | 100.36      | 109.60   |
| 1   | C     | 150 | GLN  | O-C-N     | 6.15  | 128.43      | 122.03   |
| 1   | B     | 101 | ALA  | CB-CA-C   | -6.15 | 100.23      | 110.68   |
| 2   | O     | 357 | GLY  | N-CA-C    | -6.14 | 104.34      | 112.82   |
| 2   | O     | 492 | VAL  | N-CA-C    | -6.14 | 104.75      | 110.53   |
| 2   | P     | 414 | ARG  | CD-NE-CZ  | -6.14 | 115.81      | 124.40   |
| 1   | A     | 30  | THR  | CA-CB-OG1 | -6.12 | 100.41      | 109.60   |
| 1   | F     | 155 | CYS  | O-C-N     | 6.12  | 126.75      | 121.30   |
| 1   | A     | 5   | LEU  | N-CA-C    | -6.10 | 102.08      | 109.83   |
| 1   | B     | 87  | ASN  | CA-CB-CG  | 6.10  | 118.70      | 112.60   |
| 2   | R     | 372 | LEU  | N-CA-CB   | -6.09 | 100.07      | 110.11   |
| 2   | M     | 338 | SER  | CA-C-O    | -6.08 | 114.11      | 121.05   |
| 2   | Q     | 326 | THR  | CA-CB-OG1 | -6.07 | 100.50      | 109.60   |
| 2   | O     | 509 | ASP  | CA-C-N    | 6.06  | 129.00      | 120.28   |
| 2   | O     | 509 | ASP  | C-N-CA    | 6.06  | 129.00      | 120.28   |
| 2   | Q     | 419 | LEU  | N-CA-C    | -6.05 | 102.39      | 110.55   |
| 2   | O     | 457 | ARG  | N-CA-C    | -6.04 | 102.17      | 109.83   |
| 2   | N     | 304 | ASP  | CA-CB-CG  | 6.03  | 118.63      | 112.60   |
| 1   | B     | 166 | ARG  | NE-CZ-NH1 | 6.03  | 127.53      | 121.50   |
| 2   | P     | 316 | HIS  | CA-CB-CG  | -6.02 | 107.78      | 113.80   |
| 1   | B     | 116 | ASN  | CA-CB-CG  | 6.02  | 118.62      | 112.60   |
| 2   | O     | 385 | VAL  | CA-C-O    | -6.01 | 115.30      | 121.67   |
| 2   | M     | 314 | ASN  | N-CA-C    | -6.01 | 106.11      | 113.50   |
| 1   | F     | 189 | ILE  | O-C-N     | 6.00  | 128.01      | 121.83   |
| 2   | R     | 304 | ASP  | CA-CB-CG  | -6.00 | 106.60      | 112.60   |
| 2   | R     | 420 | ASP  | CB-CA-C   | 5.99  | 117.04      | 110.15   |
| 1   | D     | 24  | GLU  | CA-CB-CG  | 5.98  | 126.06      | 114.10   |
| 2   | O     | 333 | ARG  | N-CA-C    | -5.98 | 106.12      | 113.41   |
| 2   | M     | 535 | PHE  | CA-C-O    | -5.97 | 113.61      | 121.08   |
| 1   | C     | 163 | GLN  | N-CA-C    | 5.97  | 117.54      | 109.24   |
| 2   | O     | 420 | ASP  | CB-CA-C   | 5.95  | 116.77      | 110.17   |
| 2   | M     | 337 | VAL  | CA-C-O    | -5.93 | 114.12      | 120.59   |
| 2   | M     | 420 | ASP  | O-C-N     | 5.93  | 127.88      | 121.12   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | R     | 440 | ARG  | NH1-CZ-NH2 | 5.93  | 127.01      | 119.30   |
| 2   | R     | 512 | ASN  | CA-CB-CG   | -5.91 | 106.69      | 112.60   |
| 2   | N     | 457 | ARG  | CD-NE-CZ   | 5.88  | 132.64      | 124.40   |
| 2   | O     | 340 | PRO  | CB-CA-C    | 5.88  | 118.69      | 110.98   |
| 1   | B     | 166 | ARG  | CD-NE-CZ   | 5.88  | 132.63      | 124.40   |
| 1   | A     | 52  | LEU  | CB-CA-C    | 5.87  | 123.07      | 110.45   |
| 2   | P     | 383 | ARG  | CD-NE-CZ   | -5.87 | 116.18      | 124.40   |
| 2   | M     | 316 | HIS  | O-C-N      | 5.86  | 127.81      | 121.60   |
| 2   | R     | 452 | GLY  | N-CA-C     | -5.86 | 100.38      | 112.34   |
| 1   | F     | 181 | THR  | N-CA-CB    | 5.84  | 118.55      | 109.85   |
| 2   | O     | 440 | ARG  | NH1-CZ-NH2 | 5.83  | 126.88      | 119.30   |
| 2   | P     | 514 | ASN  | OD1-CG-ND2 | -5.83 | 116.77      | 122.60   |
| 1   | F     | 125 | HIS  | CA-CB-CG   | -5.83 | 107.97      | 113.80   |
| 2   | Q     | 428 | ARG  | NE-CZ-NH2  | -5.82 | 113.96      | 119.20   |
| 1   | B     | 189 | ILE  | N-CA-CB    | 5.82  | 119.31      | 110.58   |
| 2   | P     | 376 | GLU  | O-C-N      | 5.81  | 130.17      | 123.02   |
| 2   | O     | 309 | VAL  | O-C-N      | 5.81  | 128.60      | 122.67   |
| 2   | O     | 499 | GLU  | CB-CG-CD   | 5.79  | 122.44      | 112.60   |
| 1   | A     | 57  | ASP  | CA-CB-CG   | 5.77  | 118.37      | 112.60   |
| 1   | A     | 94  | ARG  | NE-CZ-NH1  | 5.77  | 127.27      | 121.50   |
| 1   | D     | 4   | LEU  | N-CA-CB    | -5.76 | 101.23      | 110.51   |
| 1   | E     | 103 | GLU  | CA-C-O     | -5.75 | 114.38      | 121.11   |
| 2   | Q     | 387 | GLN  | CB-CG-CD   | -5.75 | 102.83      | 112.60   |
| 1   | F     | 43  | ASP  | CA-CB-CG   | -5.75 | 106.85      | 112.60   |
| 2   | M     | 428 | ARG  | CD-NE-CZ   | 5.74  | 132.44      | 124.40   |
| 2   | M     | 357 | GLY  | N-CA-C     | -5.73 | 105.20      | 112.54   |
| 2   | P     | 395 | THR  | CA-CB-OG1  | -5.73 | 101.01      | 109.60   |
| 2   | P     | 494 | SER  | N-CA-C     | -5.72 | 105.18      | 111.82   |
| 1   | C     | 32  | ASP  | CA-CB-CG   | 5.72  | 118.32      | 112.60   |
| 2   | Q     | 367 | PHE  | CA-C-O     | -5.72 | 111.08      | 120.80   |
| 2   | N     | 457 | ARG  | NE-CZ-NH2  | -5.72 | 114.05      | 119.20   |
| 1   | C     | 64  | ARG  | CD-NE-CZ   | -5.70 | 116.42      | 124.40   |
| 1   | E     | 194 | GLU  | CA-C-O     | -5.69 | 114.44      | 120.92   |
| 1   | F     | 37  | ASN  | CA-CB-CG   | -5.68 | 106.92      | 112.60   |
| 2   | R     | 314 | ASN  | OD1-CG-ND2 | 5.68  | 128.28      | 122.60   |
| 2   | O     | 383 | ARG  | N-CA-CB    | -5.68 | 100.97      | 111.53   |
| 2   | O     | 414 | ARG  | CD-NE-CZ   | -5.67 | 116.45      | 124.40   |
| 2   | M     | 372 | LEU  | N-CA-CB    | -5.67 | 100.76      | 110.11   |
| 1   | C     | 99  | PHE  | CA-CB-CG   | 5.66  | 119.46      | 113.80   |
| 2   | P     | 417 | ALA  | N-CA-C     | -5.65 | 102.65      | 109.83   |
| 1   | A     | 125 | HIS  | CA-CB-CG   | -5.65 | 108.15      | 113.80   |
| 1   | F     | 30  | THR  | CA-CB-OG1  | -5.65 | 101.13      | 109.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | O     | 533 | THR  | CA-CB-OG1  | -5.65 | 101.13      | 109.60   |
| 1   | B     | 166 | ARG  | NE-CZ-NH2  | -5.64 | 114.12      | 119.20   |
| 1   | C     | 188 | ARG  | NE-CZ-NH1  | 5.64  | 127.14      | 121.50   |
| 1   | F     | 112 | GLY  | CA-C-N     | 5.64  | 128.75      | 120.91   |
| 1   | F     | 112 | GLY  | C-N-CA     | 5.64  | 128.75      | 120.91   |
| 2   | N     | 311 | ARG  | CD-NE-CZ   | 5.63  | 132.28      | 124.40   |
| 1   | C     | 5   | LEU  | O-C-N      | 5.62  | 127.09      | 121.30   |
| 2   | O     | 489 | CYS  | CA-C-N     | 5.62  | 125.47      | 119.28   |
| 2   | O     | 489 | CYS  | C-N-CA     | 5.62  | 125.47      | 119.28   |
| 1   | C     | 162 | GLU  | CA-C-N     | 5.62  | 129.42      | 121.61   |
| 1   | C     | 162 | GLU  | C-N-CA     | 5.62  | 129.42      | 121.61   |
| 2   | O     | 528 | ARG  | NE-CZ-NH2  | -5.62 | 114.14      | 119.20   |
| 2   | R     | 385 | VAL  | CA-C-O     | -5.62 | 115.94      | 121.67   |
| 1   | C     | 99  | PHE  | N-CA-C     | -5.61 | 106.51      | 113.19   |
| 1   | C     | 70  | VAL  | CA-C-N     | 5.61  | 130.70      | 122.39   |
| 1   | C     | 70  | VAL  | C-N-CA     | 5.61  | 130.70      | 122.39   |
| 1   | C     | 181 | THR  | N-CA-CB    | 5.61  | 118.28      | 109.69   |
| 1   | E     | 99  | PHE  | CA-CB-CG   | 5.61  | 119.41      | 113.80   |
| 2   | O     | 417 | ALA  | N-CA-C     | -5.61 | 102.59      | 109.65   |
| 1   | A     | 165 | GLN  | OE1-CD-NE2 | -5.60 | 117.00      | 122.60   |
| 1   | D     | 86  | GLU  | CG-CD-OE1  | 5.59  | 131.27      | 118.40   |
| 1   | D     | 145 | PHE  | CA-CB-CG   | 5.59  | 119.39      | 113.80   |
| 2   | P     | 514 | ASN  | CB-CA-C    | 5.59  | 116.38      | 110.17   |
| 1   | A     | 171 | ILE  | N-CA-C     | 5.59  | 116.15      | 107.99   |
| 1   | F     | 5   | LEU  | O-C-N      | 5.59  | 127.68      | 121.53   |
| 2   | Q     | 522 | ARG  | CA-C-O     | -5.58 | 114.39      | 120.36   |
| 2   | O     | 458 | PRO  | CA-C-O     | -5.58 | 114.94      | 122.08   |
| 1   | B     | 4   | LEU  | N-CA-CB    | -5.57 | 101.97      | 110.49   |
| 1   | C     | 101 | ALA  | N-CA-CB    | -5.56 | 101.10      | 110.49   |
| 2   | R     | 415 | TYR  | N-CA-C     | -5.55 | 102.80      | 110.35   |
| 2   | M     | 452 | GLY  | N-CA-C     | -5.55 | 101.02      | 112.34   |
| 1   | D     | 21  | LEU  | N-CA-CB    | -5.55 | 103.22      | 110.88   |
| 1   | F     | 165 | GLN  | OE1-CD-NE2 | -5.55 | 117.05      | 122.60   |
| 1   | C     | 100 | ASP  | N-CA-C     | -5.54 | 104.24      | 108.78   |
| 1   | C     | 76  | ASN  | CA-CB-CG   | -5.54 | 107.06      | 112.60   |
| 2   | Q     | 494 | SER  | N-CA-C     | -5.54 | 105.63      | 112.38   |
| 2   | P     | 452 | GLY  | N-CA-C     | -5.52 | 101.09      | 112.34   |
| 2   | P     | 357 | GLY  | CA-C-N     | 5.51  | 128.22      | 120.28   |
| 2   | P     | 357 | GLY  | C-N-CA     | 5.51  | 128.22      | 120.28   |
| 2   | O     | 417 | ALA  | CB-CA-C    | 5.51  | 118.34      | 109.41   |
| 1   | B     | 163 | GLN  | CA-C-N     | 5.51  | 125.86      | 119.47   |
| 1   | B     | 163 | GLN  | C-N-CA     | 5.51  | 125.86      | 119.47   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | F     | 38  | ARG  | CA-CB-CG   | 5.51  | 125.11      | 114.10   |
| 1   | E     | 141 | THR  | CA-CB-OG1  | -5.50 | 101.34      | 109.60   |
| 1   | B     | 5   | LEU  | N-CA-C     | -5.50 | 102.48      | 110.08   |
| 1   | C     | 19  | ILE  | CA-CB-CG2  | 5.50  | 119.85      | 110.50   |
| 2   | Q     | 357 | GLY  | N-CA-C     | -5.50 | 105.23      | 112.82   |
| 1   | F     | 174 | ARG  | CD-NE-CZ   | -5.50 | 116.70      | 124.40   |
| 1   | A     | 141 | THR  | CA-CB-CG2  | 5.49  | 119.84      | 110.50   |
| 1   | E     | 69  | GLU  | CB-CG-CD   | 5.48  | 121.92      | 112.60   |
| 1   | D     | 159 | ASN  | OD1-CG-ND2 | -5.48 | 117.12      | 122.60   |
| 1   | E     | 76  | ASN  | CA-CB-CG   | -5.48 | 107.12      | 112.60   |
| 1   | D     | 23  | LEU  | CB-CA-C    | 5.48  | 119.94      | 110.84   |
| 2   | Q     | 505 | ILE  | N-CA-C     | 5.48  | 115.67      | 107.51   |
| 2   | N     | 483 | ASP  | CA-CB-CG   | 5.47  | 118.07      | 112.60   |
| 1   | A     | 41  | LYS  | N-CA-C     | -5.47 | 103.17      | 110.07   |
| 1   | A     | 43  | ASP  | CA-CB-CG   | -5.47 | 107.13      | 112.60   |
| 2   | O     | 313 | ARG  | NE-CZ-NH1  | 5.46  | 126.97      | 121.50   |
| 1   | D     | 66  | SER  | N-CA-CB    | 5.46  | 118.04      | 110.17   |
| 1   | D     | 28  | ASN  | O-C-N      | 5.46  | 125.99      | 121.35   |
| 2   | R     | 392 | VAL  | CA-C-O     | -5.46 | 117.17      | 120.88   |
| 2   | P     | 496 | ALA  | CA-C-N     | 5.45  | 129.18      | 121.61   |
| 2   | P     | 496 | ALA  | C-N-CA     | 5.45  | 129.18      | 121.61   |
| 2   | Q     | 354 | LEU  | CB-CA-C    | 5.45  | 118.76      | 109.72   |
| 2   | P     | 314 | ASN  | CB-CA-C    | 5.44  | 119.20      | 109.29   |
| 1   | B     | 31  | ARG  | CD-NE-CZ   | 5.44  | 132.02      | 124.40   |
| 1   | A     | 18  | HIS  | CA-CB-CG   | -5.44 | 108.36      | 113.80   |
| 1   | A     | 38  | ARG  | CD-NE-CZ   | -5.43 | 116.80      | 124.40   |
| 1   | C     | 177 | VAL  | O-C-N      | 5.43  | 128.96      | 123.20   |
| 2   | O     | 479 | TYR  | CA-C-O     | -5.43 | 115.11      | 121.46   |
| 2   | M     | 463 | PHE  | CA-C-O     | -5.42 | 114.98      | 121.11   |
| 1   | F     | 138 | HIS  | CA-C-O     | 5.42  | 127.30      | 121.44   |
| 1   | F     | 188 | ARG  | CD-NE-CZ   | -5.42 | 116.81      | 124.40   |
| 2   | R     | 508 | LEU  | N-CA-C     | -5.42 | 102.37      | 110.23   |
| 1   | E     | 111 | PRO  | CA-C-N     | 5.42  | 127.46      | 120.64   |
| 1   | E     | 111 | PRO  | C-N-CA     | 5.42  | 127.46      | 120.64   |
| 2   | Q     | 459 | ALA  | N-CA-C     | -5.42 | 102.03      | 110.10   |
| 2   | R     | 499 | GLU  | CA-CB-CG   | 5.42  | 124.93      | 114.10   |
| 1   | E     | 81  | ASP  | N-CA-C     | 5.41  | 118.10      | 111.82   |
| 2   | M     | 328 | ILE  | N-CA-C     | 5.41  | 115.55      | 110.30   |
| 2   | O     | 411 | LYS  | CB-CA-C    | -5.41 | 102.32      | 110.92   |
| 2   | R     | 497 | ASN  | CA-C-O     | 5.41  | 124.09      | 119.66   |
| 2   | O     | 314 | ASN  | CB-CA-C    | 5.40  | 119.05      | 109.65   |
| 2   | O     | 440 | ARG  | O-C-N      | 5.40  | 129.62      | 123.31   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | E     | 52  | LEU  | CB-CA-C   | 5.40  | 121.43      | 109.94   |
| 2   | R     | 463 | PHE  | O-C-N     | 5.39  | 129.85      | 123.27   |
| 1   | A     | 87  | ASN  | O-C-N     | 5.39  | 129.05      | 122.96   |
| 2   | Q     | 353 | HIS  | CA-CB-CG  | -5.39 | 108.41      | 113.80   |
| 1   | A     | 133 | ARG  | N-CA-C    | -5.38 | 102.31      | 110.28   |
| 2   | R     | 328 | ILE  | N-CA-C    | 5.38  | 116.01      | 110.36   |
| 2   | O     | 480 | PHE  | CA-C-O    | 5.38  | 126.29      | 120.43   |
| 2   | M     | 307 | ARG  | CA-C-O    | -5.37 | 114.83      | 121.06   |
| 1   | F     | 176 | GLU  | CG-CD-OE1 | 5.36  | 130.73      | 118.40   |
| 2   | R     | 326 | THR  | CA-CB-OG1 | -5.36 | 101.56      | 109.60   |
| 1   | D     | 180 | LYS  | O-C-N     | 5.36  | 130.01      | 123.21   |
| 1   | E     | 94  | ARG  | NE-CZ-NH1 | 5.36  | 126.86      | 121.50   |
| 2   | P     | 528 | ARG  | CD-NE-CZ  | 5.35  | 131.89      | 124.40   |
| 1   | E     | 41  | LYS  | N-CA-C    | -5.34 | 102.92      | 110.29   |
| 1   | D     | 106 | LEU  | N-CA-CB   | -5.34 | 101.66      | 111.37   |
| 1   | F     | 146 | ASP  | CA-CB-CG  | 5.34  | 117.94      | 112.60   |
| 2   | O     | 365 | LEU  | CA-C-O    | -5.33 | 113.04      | 118.90   |
| 1   | D     | 43  | ASP  | CA-CB-CG  | -5.33 | 107.27      | 112.60   |
| 1   | A     | 122 | MET  | CA-C-O    | -5.33 | 115.00      | 121.28   |
| 1   | B     | 139 | LEU  | O-C-N     | 5.32  | 129.42      | 123.19   |
| 2   | P     | 440 | ARG  | CB-CG-CD  | -5.32 | 99.06       | 111.30   |
| 1   | E     | 162 | GLU  | N-CA-C    | 5.32  | 117.51      | 111.02   |
| 2   | O     | 514 | ASN  | CA-CB-CG  | 5.31  | 117.91      | 112.60   |
| 2   | M     | 489 | CYS  | O-C-N     | 5.30  | 125.82      | 121.31   |
| 2   | N     | 450 | ARG  | CD-NE-CZ  | 5.29  | 131.81      | 124.40   |
| 1   | C     | 171 | ILE  | CB-CA-C   | 5.29  | 118.23      | 110.98   |
| 1   | A     | 148 | GLU  | CA-C-N    | 5.29  | 127.68      | 120.54   |
| 1   | A     | 148 | GLU  | C-N-CA    | 5.29  | 127.68      | 120.54   |
| 2   | R     | 532 | LYS  | N-CA-C    | -5.29 | 103.41      | 110.55   |
| 2   | O     | 441 | THR  | N-CA-CB   | -5.29 | 103.00      | 110.51   |
| 2   | P     | 527 | LEU  | CA-C-O    | -5.28 | 115.02      | 121.78   |
| 1   | C     | 112 | GLY  | N-CA-C    | -5.28 | 104.36      | 112.85   |
| 2   | P     | 366 | ASN  | N-CA-C    | 5.28  | 119.47      | 113.19   |
| 2   | M     | 476 | THR  | CA-CB-CG2 | 5.27  | 119.46      | 110.50   |
| 2   | Q     | 336 | LEU  | N-CA-C    | -5.27 | 103.07      | 110.50   |
| 1   | A     | 19  | ILE  | CB-CA-C   | 5.26  | 120.31      | 112.16   |
| 1   | E     | 95  | THR  | CA-C-O    | -5.25 | 115.83      | 121.45   |
| 2   | R     | 376 | GLU  | CG-CD-OE2 | -5.24 | 106.34      | 118.40   |
| 1   | F     | 133 | ARG  | N-CA-C    | -5.22 | 102.66      | 110.23   |
| 1   | E     | 84  | ASN  | N-CA-CB   | -5.22 | 101.67      | 110.49   |
| 2   | O     | 333 | ARG  | NE-CZ-NH2 | -5.21 | 114.51      | 119.20   |
| 1   | C     | 100 | ASP  | CA-C-O    | 5.20  | 120.96      | 117.94   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | R     | 480 | PHE  | CA-CB-CG  | -5.20 | 108.60      | 113.80   |
| 2   | P     | 337 | VAL  | CA-C-O    | -5.20 | 114.71      | 120.74   |
| 2   | P     | 506 | ALA  | CB-CA-C   | 5.19  | 118.31      | 109.53   |
| 1   | E     | 61  | HIS  | CA-CB-CG  | -5.19 | 108.61      | 113.80   |
| 2   | R     | 383 | ARG  | N-CA-CB   | -5.19 | 101.92      | 111.37   |
| 2   | N     | 441 | THR  | N-CA-CB   | -5.19 | 103.14      | 110.51   |
| 2   | O     | 473 | LYS  | CB-CA-C   | 5.19  | 117.62      | 109.84   |
| 2   | R     | 532 | LYS  | O-C-N     | 5.19  | 128.76      | 122.85   |
| 1   | A     | 21  | LEU  | N-CA-C    | 5.18  | 121.39      | 113.61   |
| 1   | B     | 188 | ARG  | NE-CZ-NH2 | -5.18 | 114.54      | 119.20   |
| 1   | B     | 177 | VAL  | O-C-N     | 5.17  | 128.69      | 123.20   |
| 2   | Q     | 366 | ASN  | N-CA-C    | 5.17  | 119.34      | 113.19   |
| 1   | D     | 178 | ASP  | CA-CB-CG  | -5.17 | 107.43      | 112.60   |
| 2   | P     | 457 | ARG  | N-CA-C    | -5.16 | 103.53      | 109.93   |
| 1   | B     | 43  | ASP  | CB-CA-C   | 5.16  | 119.06      | 111.17   |
| 1   | D     | 19  | ILE  | CA-CB-CG1 | 5.16  | 119.17      | 110.40   |
| 2   | Q     | 441 | THR  | N-CA-CB   | -5.16 | 102.92      | 110.97   |
| 2   | O     | 451 | ASN  | N-CA-C    | -5.15 | 99.93       | 108.12   |
| 1   | E     | 96  | ALA  | N-CA-CB   | -5.15 | 103.43      | 111.56   |
| 2   | R     | 533 | THR  | N-CA-C    | -5.15 | 103.60      | 110.55   |
| 2   | O     | 409 | ARG  | NE-CZ-NH1 | -5.14 | 116.36      | 121.50   |
| 1   | B     | 137 | ILE  | CB-CA-C   | 5.13  | 117.83      | 110.33   |
| 2   | P     | 489 | CYS  | N-CA-C    | 5.13  | 117.02      | 109.42   |
| 2   | R     | 514 | ASN  | CB-CA-C   | 5.13  | 115.25      | 110.17   |
| 1   | B     | 100 | ASP  | CA-CB-CG  | 5.13  | 117.73      | 112.60   |
| 2   | P     | 481 | GLU  | CB-CG-CD  | 5.13  | 121.33      | 112.60   |
| 2   | R     | 419 | LEU  | N-CA-C    | -5.13 | 102.93      | 110.52   |
| 2   | M     | 440 | ARG  | CB-CG-CD  | -5.13 | 99.50       | 111.30   |
| 2   | P     | 322 | PRO  | CB-CA-C   | 5.13  | 120.02      | 111.56   |
| 1   | A     | 4   | LEU  | N-CA-CB   | -5.12 | 102.65      | 110.49   |
| 1   | F     | 177 | VAL  | O-C-N     | 5.12  | 128.00      | 123.03   |
| 2   | M     | 411 | LYS  | CB-CA-C   | -5.12 | 102.25      | 110.74   |
| 2   | R     | 440 | ARG  | CB-CG-CD  | -5.11 | 99.54       | 111.30   |
| 2   | R     | 470 | ILE  | N-CA-C    | -5.11 | 106.11      | 113.07   |
| 1   | E     | 129 | SER  | CA-C-O    | -5.11 | 114.84      | 120.36   |
| 1   | C     | 95  | THR  | CA-C-O    | -5.11 | 115.99      | 121.45   |
| 1   | B     | 28  | ASN  | O-C-N     | 5.10  | 125.79      | 121.20   |
| 1   | D     | 112 | GLY  | N-CA-C    | -5.10 | 104.40      | 112.66   |
| 1   | F     | 141 | THR  | CA-CB-CG2 | 5.10  | 119.17      | 110.50   |
| 2   | R     | 347 | THR  | CA-CB-CG2 | 5.09  | 119.16      | 110.50   |
| 2   | M     | 481 | GLU  | CA-C-N    | 5.09  | 130.29      | 122.20   |
| 2   | M     | 481 | GLU  | C-N-CA    | 5.09  | 130.29      | 122.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | N     | 459 | ALA  | N-CA-C     | -5.09 | 102.85      | 110.23   |
| 2   | N     | 505 | ILE  | N-CA-C     | 5.09  | 115.67      | 107.73   |
| 2   | O     | 392 | VAL  | O-C-N      | 5.09  | 126.90      | 121.10   |
| 2   | M     | 316 | HIS  | N-CA-C     | -5.08 | 102.88      | 110.20   |
| 2   | O     | 366 | ASN  | N-CA-C     | 5.08  | 119.35      | 113.20   |
| 1   | D     | 5   | LEU  | N-CA-C     | -5.08 | 103.38      | 109.83   |
| 1   | C     | 55  | VAL  | CA-C-O     | -5.08 | 114.98      | 120.36   |
| 2   | P     | 523 | PHE  | CA-CB-CG   | 5.08  | 118.88      | 113.80   |
| 2   | N     | 357 | GLY  | N-CA-C     | -5.07 | 105.82      | 112.82   |
| 1   | B     | 21  | LEU  | N-CA-CB    | -5.07 | 103.25      | 110.80   |
| 1   | D     | 41  | LYS  | N-CA-C     | -5.07 | 103.30      | 110.29   |
| 1   | B     | 64  | ARG  | NE-CZ-NH2  | 5.06  | 123.75      | 119.20   |
| 1   | E     | 116 | ASN  | N-CA-C     | -5.06 | 103.92      | 110.19   |
| 2   | Q     | 512 | ASN  | N-CA-CB    | -5.06 | 102.98      | 110.61   |
| 2   | O     | 457 | ARG  | CA-CB-CG   | 5.05  | 124.21      | 114.10   |
| 1   | C     | 137 | ILE  | CB-CA-C    | 5.05  | 117.71      | 110.33   |
| 1   | F     | 143 | LEU  | CA-C-N     | 5.05  | 131.29      | 122.81   |
| 1   | F     | 143 | LEU  | C-N-CA     | 5.05  | 131.29      | 122.81   |
| 2   | N     | 324 | TYR  | CA-C-N     | 5.05  | 128.39      | 120.82   |
| 2   | N     | 324 | TYR  | C-N-CA     | 5.05  | 128.39      | 120.82   |
| 2   | M     | 356 | PHE  | CA-CB-CG   | 5.04  | 118.84      | 113.80   |
| 2   | P     | 478 | LEU  | CB-CA-C    | 5.04  | 117.96      | 109.48   |
| 1   | B     | 27  | GLY  | N-CA-C     | -5.04 | 107.86      | 115.32   |
| 1   | D     | 94  | ARG  | CG-CD-NE   | 5.04  | 123.10      | 112.00   |
| 1   | F     | 95  | THR  | CA-CB-OG1  | -5.04 | 102.04      | 109.60   |
| 2   | P     | 524 | ASP  | CA-CB-CG   | 5.04  | 117.64      | 112.60   |
| 2   | M     | 390 | LYS  | CA-CB-CG   | 5.04  | 124.17      | 114.10   |
| 1   | B     | 135 | ILE  | CA-C-N     | 5.04  | 127.44      | 120.29   |
| 1   | B     | 135 | ILE  | C-N-CA     | 5.04  | 127.44      | 120.29   |
| 2   | M     | 451 | ASN  | OD1-CG-ND2 | 5.03  | 127.63      | 122.60   |
| 1   | B     | 30  | THR  | CA-CB-OG1  | -5.03 | 102.06      | 109.60   |
| 2   | O     | 383 | ARG  | CD-NE-CZ   | -5.03 | 117.36      | 124.40   |
| 2   | O     | 499 | GLU  | CG-CD-OE1  | 5.03  | 129.96      | 118.40   |
| 2   | R     | 428 | ARG  | NE-CZ-NH2  | -5.03 | 114.67      | 119.20   |
| 1   | D     | 131 | PHE  | CA-CB-CG   | 5.03  | 118.83      | 113.80   |
| 2   | O     | 443 | LYS  | O-C-N      | 5.02  | 125.85      | 121.18   |
| 2   | O     | 411 | LYS  | O-C-N      | 5.02  | 127.45      | 122.08   |
| 2   | N     | 440 | ARG  | CB-CG-CD   | -5.02 | 99.76       | 111.30   |
| 1   | A     | 99  | PHE  | CA-CB-CG   | 5.01  | 118.81      | 113.80   |
| 1   | E     | 28  | ASN  | O-C-N      | 5.01  | 125.46      | 121.55   |
| 2   | R     | 314 | ASN  | N-CA-C     | -5.01 | 107.20      | 113.72   |
| 2   | R     | 367 | PHE  | CA-C-O     | -5.01 | 112.29      | 120.80   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 32  | ASP  | O-C-N     | 5.00  | 127.44      | 122.08   |
| 1   | A     | 97  | THR  | CA-CB-OG1 | -5.00 | 102.10      | 109.60   |
| 2   | P     | 428 | ARG  | CG-CD-NE  | 5.00  | 123.01      | 112.00   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | B     | 184 | ARG  | Sidechain |
| 2   | R     | 407 | 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     | 62      | 0            |
| 1   | B     | 1571  | 0        | 1499     | 50      | 0            |
| 1   | C     | 1571  | 0        | 1499     | 64      | 0            |
| 1   | D     | 1571  | 0        | 1499     | 45      | 0            |
| 1   | E     | 1571  | 0        | 1499     | 72      | 0            |
| 1   | F     | 1571  | 0        | 1499     | 79      | 0            |
| 2   | M     | 1840  | 0        | 1793     | 64      | 0            |
| 2   | N     | 1840  | 0        | 1793     | 45      | 0            |
| 2   | O     | 1840  | 0        | 1793     | 58      | 0            |
| 2   | P     | 1840  | 0        | 1793     | 52      | 0            |
| 2   | Q     | 1840  | 0        | 1793     | 61      | 0            |
| 2   | R     | 1840  | 0        | 1793     | 73      | 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        | 1       | 0            |
| 4   | O     | 4     | 0        | 5        | 0       | 0            |
| 4   | P     | 4     | 0        | 5        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | Q     | 4     | 0        | 5        | 0       | 0            |
| 4   | R     | 4     | 0        | 5        | 0       | 0            |
| 5   | M     | 11    | 0        | 3        | 0       | 0            |
| 5   | N     | 11    | 0        | 3        | 1       | 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     | 79    | 0        | 0        | 1       | 0            |
| 6   | B     | 78    | 0        | 0        | 1       | 0            |
| 6   | C     | 76    | 0        | 0        | 2       | 0            |
| 6   | D     | 79    | 0        | 0        | 0       | 0            |
| 6   | E     | 81    | 0        | 0        | 0       | 0            |
| 6   | F     | 75    | 0        | 0        | 1       | 0            |
| 6   | M     | 155   | 0        | 0        | 3       | 0            |
| 6   | N     | 163   | 0        | 0        | 5       | 0            |
| 6   | O     | 158   | 0        | 0        | 6       | 0            |
| 6   | P     | 149   | 0        | 0        | 5       | 0            |
| 6   | Q     | 160   | 0        | 0        | 6       | 0            |
| 6   | R     | 163   | 0        | 0        | 4       | 0            |
| All | All   | 21978 | 0        | 19800    | 645     | 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 16.

All (645) 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:B:165:GLN:H    | 1:B:165:GLN:NE2  | 1.34                     | 1.22              |
| 1:E:165:GLN:H    | 1:E:165:GLN:NE2  | 1.36                     | 1.21              |
| 1:E:165:GLN:HE21 | 1:E:165:GLN:N    | 1.40                     | 1.16              |
| 2:R:497:ASN:ND2  | 2:R:499:GLU:H    | 1.48                     | 1.11              |
| 1:A:134:GLY:CA   | 2:M:326:THR:HG22 | 1.88                     | 1.03              |
| 1:B:165:GLN:N    | 1:B:165:GLN:HE21 | 1.60                     | 1.00              |
| 1:B:165:GLN:H    | 1:B:165:GLN:HE21 | 0.96                     | 0.94              |
| 1:B:165:GLN:NE2  | 1:B:165:GLN:N    | 2.18                     | 0.90              |
| 1:A:134:GLY:HA3  | 2:M:326:THR:HG22 | 1.54                     | 0.89              |
| 1:E:176:GLU:OE2  | 1:E:179:GLY:HA2  | 1.73                     | 0.88              |
| 2:R:497:ASN:C    | 2:R:497:ASN:HD22 | 1.83                     | 0.87              |
| 1:A:163:GLN:HB3  | 1:A:165:GLN:NE2  | 1.90                     | 0.86              |
| 2:M:497:ASN:ND2  | 2:M:499:GLU:H    | 1.73                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:67:PHE:HZ    | 1:B:94:ARG:HD2   | 1.40                     | 0.84              |
| 2:R:361:HIS:H    | 2:R:361:HIS:CD2  | 1.90                     | 0.84              |
| 1:D:67:PHE:HZ    | 1:D:94:ARG:HD2   | 1.40                     | 0.84              |
| 2:R:497:ASN:HD22 | 2:R:498:PRO:N    | 1.78                     | 0.82              |
| 1:D:67:PHE:CZ    | 1:D:94:ARG:HD2   | 2.15                     | 0.82              |
| 2:M:390:LYS:HD2  | 6:M:643:HOH:O    | 1.80                     | 0.81              |
| 1:E:51:LEU:HD12  | 1:E:106:LEU:HD23 | 1.62                     | 0.80              |
| 2:M:508:LEU:HD23 | 2:P:488:MET:HE1  | 1.64                     | 0.80              |
| 1:B:33:GLN:HG2   | 1:B:85:LEU:HD12  | 1.61                     | 0.80              |
| 1:E:19:ILE:HD11  | 2:Q:408:TYR:HD1  | 1.47                     | 0.80              |
| 2:R:497:ASN:ND2  | 2:R:499:GLU:N    | 2.28                     | 0.80              |
| 2:P:390:LYS:HD2  | 6:P:683:HOH:O    | 1.82                     | 0.79              |
| 2:Q:390:LYS:HD3  | 6:Q:670:HOH:O    | 1.81                     | 0.79              |
| 1:F:165:GLN:H    | 1:F:165:GLN:NE2  | 1.80                     | 0.79              |
| 2:N:497:ASN:ND2  | 2:N:499:GLU:HB2  | 1.97                     | 0.79              |
| 2:R:361:HIS:H    | 2:R:361:HIS:HD2  | 1.29                     | 0.79              |
| 2:Q:497:ASN:ND2  | 2:Q:499:GLU:OE1  | 2.13                     | 0.79              |
| 2:N:307:ARG:HG2  | 2:N:533:THR:HG22 | 1.63                     | 0.79              |
| 1:D:114:VAL:HG23 | 1:D:122:MET:HE3  | 1.65                     | 0.79              |
| 2:Q:390:LYS:HE2  | 6:Q:747:HOH:O    | 1.83                     | 0.78              |
| 2:R:497:ASN:HD21 | 2:R:499:GLU:H    | 1.32                     | 0.78              |
| 2:N:497:ASN:HD22 | 2:N:499:GLU:H    | 1.31                     | 0.78              |
| 2:R:315:TRP:HZ2  | 2:R:503:GLN:NE2  | 1.82                     | 0.77              |
| 1:A:114:VAL:HG23 | 1:A:122:MET:HE3  | 1.66                     | 0.77              |
| 2:R:497:ASN:HD22 | 2:R:499:GLU:H    | 1.30                     | 0.77              |
| 2:Q:361:HIS:CD2  | 2:Q:361:HIS:H    | 2.04                     | 0.75              |
| 1:B:176:GLU:HG3  | 1:B:180:LYS:C    | 2.10                     | 0.75              |
| 1:A:78:GLU:HG2   | 2:M:301:PRO:CB   | 2.16                     | 0.74              |
| 1:A:176:GLU:HG3  | 1:A:180:LYS:O    | 1.87                     | 0.74              |
| 1:D:180:LYS:HG3  | 1:D:181:THR:N    | 2.03                     | 0.74              |
| 2:Q:522:ARG:NH1  | 6:Q:691:HOH:O    | 2.20                     | 0.74              |
| 2:M:361:HIS:H    | 2:M:361:HIS:CD2  | 2.04                     | 0.74              |
| 2:Q:497:ASN:C    | 2:Q:497:ASN:HD22 | 1.92                     | 0.73              |
| 2:R:315:TRP:HZ2  | 2:R:503:GLN:HE21 | 1.35                     | 0.73              |
| 1:E:98:THR:O     | 1:E:102:GLY:HA2  | 1.89                     | 0.73              |
| 2:P:361:HIS:H    | 2:P:361:HIS:CD2  | 2.07                     | 0.73              |
| 1:A:67:PHE:HZ    | 1:A:94:ARG:HD2   | 1.54                     | 0.73              |
| 1:D:19:ILE:HD11  | 2:P:408:TYR:HD2  | 1.54                     | 0.73              |
| 2:P:497:ASN:HD22 | 2:P:499:GLU:H    | 1.37                     | 0.72              |
| 1:A:134:GLY:HA2  | 2:M:326:THR:HG22 | 1.68                     | 0.72              |
| 2:N:489:CYS:O    | 2:N:493:LYS:HG3  | 1.89                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:307:ARG:HG2  | 2:M:533:THR:HG22 | 1.72                     | 0.71              |
| 2:Q:416:LEU:HD23 | 2:Q:416:LEU:C    | 2.15                     | 0.71              |
| 2:M:497:ASN:HD22 | 2:M:499:GLU:H    | 1.37                     | 0.71              |
| 1:C:165:GLN:H    | 1:C:165:GLN:NE2  | 1.88                     | 0.71              |
| 1:D:165:GLN:NE2  | 1:D:165:GLN:H    | 1.87                     | 0.71              |
| 1:E:180:LYS:HG3  | 1:E:181:THR:N    | 2.05                     | 0.71              |
| 2:R:307:ARG:HG2  | 2:R:533:THR:HG22 | 1.73                     | 0.71              |
| 1:C:52:LEU:C     | 1:C:52:LEU:HD22  | 2.16                     | 0.71              |
| 1:B:67:PHE:CZ    | 1:B:94:ARG:HD2   | 2.25                     | 0.71              |
| 2:O:416:LEU:C    | 2:O:416:LEU:HD23 | 2.14                     | 0.71              |
| 1:E:67:PHE:HZ    | 1:E:94:ARG:HD2   | 1.56                     | 0.71              |
| 2:M:360:ASP:OD2  | 2:M:428:ARG:HD2  | 1.91                     | 0.70              |
| 2:N:359:HIS:O    | 2:N:366:ASN:HB3  | 1.92                     | 0.70              |
| 2:M:310:ILE:HD12 | 2:O:453:PRO:HB2  | 1.72                     | 0.70              |
| 1:B:163:GLN:HB3  | 1:B:165:GLN:NE2  | 2.06                     | 0.70              |
| 1:C:54:GLN:HG3   | 1:C:184:ARG:NH2  | 2.07                     | 0.70              |
| 1:F:70:VAL:HG21  | 1:F:106:LEU:HD21 | 1.74                     | 0.69              |
| 1:B:176:GLU:HG3  | 1:B:180:LYS:O    | 1.91                     | 0.69              |
| 1:C:114:VAL:HG23 | 1:C:122:MET:HE3  | 1.73                     | 0.69              |
| 1:C:41:LYS:HD2   | 1:C:88:ALA:HA    | 1.74                     | 0.69              |
| 1:C:131:PHE:O    | 1:C:132:ALA:HB2  | 1.92                     | 0.69              |
| 1:F:163:GLN:HB3  | 1:F:165:GLN:NE2  | 2.08                     | 0.69              |
| 2:N:361:HIS:CD2  | 2:N:361:HIS:H    | 2.11                     | 0.69              |
| 1:B:163:GLN:HB3  | 1:B:165:GLN:HE22 | 1.58                     | 0.68              |
| 2:N:494:SER:O    | 6:N:780:HOH:O    | 2.10                     | 0.68              |
| 2:O:361:HIS:H    | 2:O:361:HIS:CD2  | 2.12                     | 0.68              |
| 1:E:19:ILE:HG22  | 1:E:26:ALA:HB1   | 1.76                     | 0.68              |
| 1:E:110:LYS:NZ   | 1:E:183:TYR:OH   | 2.27                     | 0.68              |
| 1:A:67:PHE:CZ    | 1:A:94:ARG:HD2   | 2.30                     | 0.67              |
| 1:F:188:ARG:HG3  | 1:F:188:ARG:HH11 | 1.59                     | 0.67              |
| 1:F:48:HIS:C     | 1:F:180:LYS:NZ   | 2.53                     | 0.67              |
| 1:B:19:ILE:HG22  | 1:B:26:ALA:HB1   | 1.77                     | 0.67              |
| 1:F:163:GLN:HB3  | 1:F:165:GLN:HE21 | 1.58                     | 0.67              |
| 2:R:315:TRP:CZ2  | 2:R:503:GLN:NE2  | 2.62                     | 0.67              |
| 2:M:315:TRP:HZ2  | 2:M:503:GLN:HE21 | 1.44                     | 0.66              |
| 2:Q:388:TYR:OH   | 6:Q:621:HOH:O    | 2.13                     | 0.66              |
| 1:A:165:GLN:CD   | 1:A:165:GLN:H    | 2.04                     | 0.66              |
| 2:P:416:LEU:C    | 2:P:416:LEU:HD23 | 2.20                     | 0.66              |
| 1:E:33:GLN:HG2   | 1:E:85:LEU:HD12  | 1.78                     | 0.66              |
| 2:N:406:GLY:O    | 2:N:447:TYR:HD2  | 1.78                     | 0.65              |
| 1:C:16:TYR:O     | 1:C:19:ILE:HG23  | 1.96                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:176:GLU:HG3  | 1:C:180:LYS:O    | 1.95                     | 0.65              |
| 2:O:522:ARG:NH1  | 6:O:716:HOH:O    | 2.18                     | 0.65              |
| 1:E:19:ILE:HG21  | 2:Q:410:HIS:HB2  | 1.78                     | 0.65              |
| 1:C:65:ASP:OD2   | 1:C:133:ARG:HD3  | 1.96                     | 0.65              |
| 1:B:98:THR:O     | 1:B:102:GLY:HA2  | 1.97                     | 0.65              |
| 1:E:39:LEU:CD1   | 1:E:106:LEU:HD11 | 2.27                     | 0.65              |
| 1:C:177:VAL:O    | 1:C:180:LYS:HB3  | 1.96                     | 0.65              |
| 1:E:19:ILE:O     | 2:Q:426:VAL:HG21 | 1.95                     | 0.65              |
| 1:D:168:GLU:HA   | 1:D:171:ILE:HD12 | 1.78                     | 0.65              |
| 1:F:177:VAL:HG12 | 1:F:178:ASP:OD2  | 1.97                     | 0.65              |
| 1:B:6:PRO:HB2    | 2:N:503:GLN:HE22 | 1.63                     | 0.64              |
| 1:A:163:GLN:HG3  | 1:C:61:HIS:ND1   | 2.12                     | 0.64              |
| 1:C:110:LYS:NZ   | 1:C:147:ASP:OD1  | 2.31                     | 0.64              |
| 1:F:147:ASP:OD2  | 1:F:174:ARG:HD2  | 1.97                     | 0.64              |
| 2:R:415:TYR:CE1  | 2:R:416:LEU:CD2  | 2.81                     | 0.63              |
| 2:Q:364:LEU:HD22 | 2:Q:440:ARG:HG2  | 1.80                     | 0.63              |
| 2:O:390:LYS:HE2  | 6:O:798:HOH:O    | 1.99                     | 0.63              |
| 2:R:522:ARG:NH1  | 6:R:812:HOH:O    | 2.32                     | 0.63              |
| 2:R:473:LYS:NZ   | 6:R:859:HOH:O    | 2.32                     | 0.63              |
| 1:A:134:GLY:HA3  | 2:M:326:THR:CG2  | 2.27                     | 0.62              |
| 2:O:356:PHE:CD1  | 2:O:428:ARG:HD3  | 2.34                     | 0.62              |
| 1:D:70:VAL:HG21  | 1:D:106:LEU:HD21 | 1.80                     | 0.62              |
| 1:A:78:GLU:CG    | 2:M:301:PRO:HG3  | 2.29                     | 0.62              |
| 2:Q:359:HIS:O    | 2:Q:366:ASN:HB3  | 1.99                     | 0.62              |
| 1:F:98:THR:OG1   | 1:F:102:GLY:N    | 2.31                     | 0.62              |
| 2:M:361:HIS:H    | 2:M:361:HIS:HD2  | 1.43                     | 0.62              |
| 1:F:168:GLU:HA   | 1:F:171:ILE:HD12 | 1.81                     | 0.62              |
| 1:E:64:ARG:NE    | 1:E:100:ASP:O    | 2.31                     | 0.62              |
| 1:B:19:ILE:HD11  | 2:N:408:TYR:HD1  | 1.65                     | 0.62              |
| 2:P:383:ARG:NH2  | 2:P:391:PRO:HG3  | 2.14                     | 0.62              |
| 1:C:180:LYS:HD2  | 1:C:181:THR:H    | 1.65                     | 0.61              |
| 1:F:50:LEU:O     | 1:F:182:ALA:HA   | 2.00                     | 0.61              |
| 1:A:163:GLN:HB3  | 1:A:165:GLN:HE22 | 1.62                     | 0.61              |
| 1:A:133:ARG:HG3  | 2:M:326:THR:HG21 | 1.81                     | 0.61              |
| 1:D:24:GLU:O     | 1:D:27:GLY:N     | 2.33                     | 0.61              |
| 1:F:177:VAL:O    | 1:F:180:LYS:HB3  | 2.01                     | 0.61              |
| 2:N:400:TRP:HA   | 2:N:425:GLY:O    | 1.99                     | 0.61              |
| 1:E:19:ILE:HD11  | 2:Q:408:TYR:CD1  | 2.33                     | 0.61              |
| 2:Q:315:TRP:HZ2  | 2:Q:503:GLN:NE2  | 1.99                     | 0.61              |
| 1:A:19:ILE:O     | 2:M:426:VAL:HG21 | 2.01                     | 0.61              |
| 2:N:315:TRP:HZ2  | 2:N:503:GLN:HE21 | 1.48                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:361:HIS:H    | 2:N:361:HIS:HD2  | 1.48                     | 0.61              |
| 2:Q:376:GLU:O    | 2:Q:442:ILE:HA   | 2.01                     | 0.60              |
| 2:M:364:LEU:HD22 | 2:M:440:ARG:HD3  | 1.83                     | 0.60              |
| 1:C:44:ALA:O     | 1:C:48:HIS:NE2   | 2.22                     | 0.60              |
| 1:F:77:GLY:O     | 1:F:114:VAL:HG12 | 2.01                     | 0.60              |
| 2:Q:315:TRP:HZ2  | 2:Q:503:GLN:HE21 | 1.49                     | 0.60              |
| 2:O:359:HIS:O    | 2:O:366:ASN:HB3  | 2.02                     | 0.60              |
| 2:R:400:TRP:HA   | 2:R:425:GLY:O    | 2.02                     | 0.60              |
| 1:F:64:ARG:NE    | 1:F:100:ASP:O    | 2.30                     | 0.60              |
| 1:F:180:LYS:HD2  | 1:F:181:THR:N    | 2.16                     | 0.60              |
| 1:C:180:LYS:HD2  | 1:C:181:THR:N    | 2.16                     | 0.59              |
| 1:E:61:HIS:ND1   | 1:F:163:GLN:HG3  | 2.17                     | 0.59              |
| 2:M:497:ASN:HD22 | 2:M:498:PRO:N    | 2.01                     | 0.59              |
| 1:C:100:ASP:N    | 1:C:100:ASP:OD1  | 2.35                     | 0.59              |
| 1:D:28:ASN:HB3   | 1:D:29:PRO:HD2   | 1.84                     | 0.59              |
| 2:R:383:ARG:HD2  | 2:R:436:TYR:CZ   | 2.38                     | 0.59              |
| 2:R:497:ASN:HD22 | 2:R:499:GLU:N    | 1.96                     | 0.59              |
| 1:F:67:PHE:CZ    | 1:F:94:ARG:HD2   | 2.37                     | 0.59              |
| 1:A:144:TYR:CE1  | 1:A:158:LEU:HD13 | 2.38                     | 0.59              |
| 1:B:114:VAL:HG23 | 1:B:122:MET:HE3  | 1.84                     | 0.59              |
| 1:F:165:GLN:H    | 1:F:165:GLN:CD   | 2.11                     | 0.59              |
| 2:Q:497:ASN:ND2  | 2:Q:499:GLU:H    | 2.01                     | 0.58              |
| 2:Q:361:HIS:H    | 2:Q:361:HIS:HD2  | 1.51                     | 0.58              |
| 2:R:478:LEU:C    | 2:R:478:LEU:HD23 | 2.28                     | 0.58              |
| 2:R:497:ASN:ND2  | 2:R:497:ASN:C    | 2.55                     | 0.58              |
| 2:Q:362:ASP:OD1  | 2:Q:440:ARG:HD3  | 2.04                     | 0.58              |
| 2:R:497:ASN:ND2  | 2:R:499:GLU:OE1  | 2.36                     | 0.58              |
| 1:F:74:ASP:HB2   | 6:F:690:HOH:O    | 2.04                     | 0.58              |
| 2:P:361:HIS:H    | 2:P:361:HIS:HD2  | 1.49                     | 0.58              |
| 2:Q:405:GLY:HA3  | 6:Q:673:HOH:O    | 2.03                     | 0.58              |
| 2:P:416:LEU:HD23 | 2:P:417:ALA:N    | 2.19                     | 0.58              |
| 1:E:24:GLU:O     | 1:E:27:GLY:N     | 2.35                     | 0.58              |
| 1:E:131:PHE:CE2  | 1:E:138:HIS:HB3  | 2.39                     | 0.58              |
| 2:R:406:GLY:O    | 2:R:447:TYR:HD1  | 1.86                     | 0.58              |
| 1:F:44:ALA:O     | 1:F:48:HIS:NE2   | 2.32                     | 0.58              |
| 2:N:390:LYS:CD   | 6:N:743:HOH:O    | 2.52                     | 0.58              |
| 1:F:176:GLU:HG3  | 1:F:180:LYS:N    | 2.18                     | 0.58              |
| 2:O:406:GLY:O    | 2:O:447:TYR:HD1  | 1.87                     | 0.57              |
| 1:D:19:ILE:O     | 2:P:426:VAL:HG21 | 2.04                     | 0.57              |
| 1:D:177:VAL:O    | 1:D:180:LYS:HB3  | 2.05                     | 0.57              |
| 1:A:98:THR:O     | 1:A:102:GLY:HA2  | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:364:LEU:HD22 | 2:M:440:ARG:CD   | 2.35                     | 0.57              |
| 2:M:522:ARG:NH1  | 6:M:664:HOH:O    | 2.29                     | 0.57              |
| 2:Q:497:ASN:HD22 | 2:Q:498:PRO:N    | 2.01                     | 0.57              |
| 1:D:19:ILE:HG21  | 2:P:410:HIS:HB2  | 1.87                     | 0.57              |
| 2:N:478:LEU:C    | 2:N:478:LEU:HD23 | 2.28                     | 0.57              |
| 1:D:19:ILE:HG22  | 1:D:26:ALA:HB1   | 1.85                     | 0.57              |
| 1:E:168:GLU:HA   | 1:E:171:ILE:HD12 | 1.87                     | 0.57              |
| 1:F:35:ILE:HG22  | 1:F:94:ARG:HG3   | 1.87                     | 0.57              |
| 1:D:64:ARG:NE    | 1:D:100:ASP:O    | 2.37                     | 0.57              |
| 1:E:56:TYR:CE1   | 1:E:62:LEU:HD23  | 2.40                     | 0.57              |
| 1:E:131:PHE:CD2  | 1:E:138:HIS:HB3  | 2.40                     | 0.56              |
| 1:F:176:GLU:HG2  | 1:F:179:GLY:HA2  | 1.87                     | 0.56              |
| 1:A:176:GLU:HG3  | 1:A:180:LYS:C    | 2.30                     | 0.56              |
| 1:E:41:LYS:HD2   | 1:E:88:ALA:HA    | 1.85                     | 0.56              |
| 1:A:134:GLY:CA   | 2:M:326:THR:CG2  | 2.76                     | 0.56              |
| 1:A:176:GLU:OE2  | 1:A:179:GLY:HA2  | 2.05                     | 0.56              |
| 2:N:497:ASN:ND2  | 2:N:499:GLU:H    | 1.98                     | 0.56              |
| 1:F:48:HIS:O     | 1:F:180:LYS:NZ   | 2.38                     | 0.56              |
| 1:F:74:ASP:HB3   | 1:F:89:PHE:CE2   | 2.40                     | 0.56              |
| 2:P:497:ASN:ND2  | 2:P:499:GLU:H    | 2.02                     | 0.56              |
| 1:A:176:GLU:HA   | 1:A:180:LYS:O    | 2.05                     | 0.56              |
| 2:O:497:ASN:ND2  | 2:O:499:GLU:H    | 2.02                     | 0.56              |
| 2:Q:416:LEU:HD23 | 2:Q:417:ALA:N    | 2.20                     | 0.56              |
| 1:F:18:HIS:CE1   | 1:F:99:PHE:HE1   | 2.23                     | 0.56              |
| 1:F:176:GLU:HG3  | 1:F:180:LYS:O    | 2.06                     | 0.56              |
| 2:M:497:ASN:HD22 | 2:M:497:ASN:C    | 2.13                     | 0.56              |
| 2:Q:536:GLU:HB2  | 6:Q:723:HOH:O    | 2.05                     | 0.56              |
| 2:N:497:ASN:HD22 | 2:N:499:GLU:N    | 2.03                     | 0.56              |
| 2:O:361:HIS:HD2  | 6:O:766:HOH:O    | 1.89                     | 0.56              |
| 1:F:110:LYS:NZ   | 1:F:147:ASP:OD1  | 2.39                     | 0.55              |
| 1:F:157:VAL:O    | 1:F:160:LEU:HB2  | 2.06                     | 0.55              |
| 2:R:313:ARG:O    | 2:R:318:LYS:HD3  | 2.07                     | 0.55              |
| 2:M:399:MET:HA   | 2:M:462:HIS:O    | 2.05                     | 0.55              |
| 1:D:51:LEU:O     | 1:D:105:THR:HA   | 2.05                     | 0.55              |
| 2:O:307:ARG:HG2  | 2:O:533:THR:HG22 | 1.89                     | 0.55              |
| 1:F:50:LEU:HD12  | 1:F:51:LEU:N     | 2.22                     | 0.55              |
| 1:A:78:GLU:CD    | 2:M:301:PRO:HG3  | 2.32                     | 0.55              |
| 2:P:307:ARG:HG2  | 2:P:533:THR:HG22 | 1.88                     | 0.55              |
| 1:A:78:GLU:HG2   | 2:M:301:PRO:HB2  | 1.87                     | 0.55              |
| 1:B:190:GLN:HG3  | 2:N:333:ARG:HG2  | 1.88                     | 0.55              |
| 2:R:314:ASN:OD1  | 2:R:318:LYS:HE2  | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:39:LEU:HD13  | 1:E:106:LEU:HD11 | 1.88                     | 0.54              |
| 2:N:497:ASN:HD21 | 2:N:499:GLU:HB2  | 1.70                     | 0.54              |
| 1:E:67:PHE:CZ    | 1:E:94:ARG:HD2   | 2.41                     | 0.54              |
| 1:F:54:GLN:HG3   | 1:F:184:ARG:HH22 | 1.72                     | 0.54              |
| 2:R:484:PRO:O    | 2:R:488:MET:HE3  | 2.06                     | 0.54              |
| 1:E:19:ILE:CG2   | 2:Q:410:HIS:HB2  | 2.36                     | 0.54              |
| 2:N:364:LEU:HD22 | 2:N:440:ARG:HD3  | 1.87                     | 0.54              |
| 2:O:376:GLU:O    | 2:O:442:ILE:HA   | 2.06                     | 0.54              |
| 2:P:431:THR:HG22 | 2:P:437:TYR:HB3  | 1.90                     | 0.54              |
| 1:E:65:ASP:OD2   | 1:E:133:ARG:HD3  | 2.07                     | 0.54              |
| 1:E:114:VAL:HG23 | 1:E:122:MET:HE3  | 1.88                     | 0.54              |
| 1:A:69:GLU:OE1   | 2:M:473:LYS:HE2  | 2.07                     | 0.54              |
| 2:Q:315:TRP:CZ2  | 2:Q:503:GLN:NE2  | 2.75                     | 0.54              |
| 2:R:405:GLY:HA3  | 6:R:791:HOH:O    | 2.07                     | 0.54              |
| 1:C:19:ILE:O     | 2:O:426:VAL:HG21 | 2.08                     | 0.54              |
| 1:D:70:VAL:HG11  | 1:D:106:LEU:HD21 | 1.89                     | 0.54              |
| 1:F:98:THR:O     | 1:F:102:GLY:HA2  | 2.08                     | 0.54              |
| 2:N:486:ILE:HB   | 2:N:487:PRO:HD3  | 1.89                     | 0.54              |
| 1:E:92:PHE:CD1   | 2:Q:349:PRO:HG3  | 2.43                     | 0.54              |
| 1:A:100:ASP:N    | 1:A:100:ASP:OD1  | 2.41                     | 0.54              |
| 1:B:176:GLU:HG2  | 1:B:180:LYS:N    | 2.23                     | 0.54              |
| 2:M:448:PRO:HB2  | 2:P:516:MET:HA   | 1.90                     | 0.54              |
| 1:C:52:LEU:HD21  | 1:C:184:ARG:NH1  | 2.23                     | 0.53              |
| 2:P:360:ASP:HB3  | 2:P:428:ARG:HG3  | 1.89                     | 0.53              |
| 1:A:143:LEU:C    | 1:A:143:LEU:HD23 | 2.33                     | 0.53              |
| 2:R:361:HIS:CD2  | 2:R:361:HIS:N    | 2.62                     | 0.53              |
| 2:R:487:PRO:O    | 2:R:493:LYS:HD3  | 2.09                     | 0.53              |
| 2:P:406:GLY:O    | 2:P:447:TYR:HD1  | 1.92                     | 0.53              |
| 2:R:399:MET:HA   | 2:R:462:HIS:O    | 2.08                     | 0.53              |
| 1:F:114:VAL:HG23 | 1:F:122:MET:CE   | 2.39                     | 0.53              |
| 1:C:64:ARG:NE    | 1:C:100:ASP:O    | 2.38                     | 0.53              |
| 1:D:153:ALA:C    | 1:D:154:LYS:HE3  | 2.33                     | 0.53              |
| 1:F:54:GLN:HG3   | 1:F:184:ARG:NH2  | 2.23                     | 0.53              |
| 1:D:51:LEU:HD11  | 1:D:126:ILE:HD12 | 1.91                     | 0.53              |
| 1:B:51:LEU:HD11  | 1:B:126:ILE:HD12 | 1.89                     | 0.53              |
| 1:C:74:ASP:C     | 1:C:74:ASP:OD1   | 2.52                     | 0.53              |
| 1:E:177:VAL:HG12 | 1:E:178:ASP:OD2  | 2.09                     | 0.53              |
| 2:Q:400:TRP:HA   | 2:Q:425:GLY:O    | 2.08                     | 0.53              |
| 2:M:335:ALA:HB2  | 2:O:328:ILE:HD12 | 1.90                     | 0.53              |
| 1:C:35:ILE:HG21  | 1:C:92:PHE:HE2   | 1.74                     | 0.53              |
| 2:P:376:GLU:O    | 2:P:442:ILE:HA   | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:100:ASP:N    | 1:F:100:ASP:OD1  | 2.41                     | 0.52              |
| 1:A:163:GLN:HB3  | 1:A:165:GLN:HE21 | 1.70                     | 0.52              |
| 1:F:67:PHE:HZ    | 1:F:94:ARG:HD2   | 1.72                     | 0.52              |
| 1:B:131:PHE:CD2  | 1:B:138:HIS:HB3  | 2.44                     | 0.52              |
| 2:R:522:ARG:NE   | 2:R:524:ASP:OD1  | 2.41                     | 0.52              |
| 2:O:400:TRP:HA   | 2:O:425:GLY:O    | 2.09                     | 0.52              |
| 1:C:54:GLN:HG3   | 1:C:184:ARG:HH22 | 1.75                     | 0.52              |
| 2:O:399:MET:HA   | 2:O:462:HIS:O    | 2.09                     | 0.52              |
| 2:O:407:ARG:NH1  | 2:O:417:ALA:O    | 2.36                     | 0.52              |
| 2:O:356:PHE:CE1  | 2:O:428:ARG:HD3  | 2.45                     | 0.52              |
| 1:F:131:PHE:O    | 1:F:132:ALA:HB2  | 2.09                     | 0.52              |
| 1:F:31:ARG:NH1   | 2:R:428:ARG:HG2  | 2.24                     | 0.51              |
| 2:R:304:ASP:HB2  | 2:R:343:ILE:HB   | 1.92                     | 0.51              |
| 1:A:4:LEU:HB3    | 2:M:387:GLN:HB3  | 1.92                     | 0.51              |
| 2:M:473:LYS:NZ   | 6:M:651:HOH:O    | 2.38                     | 0.51              |
| 2:N:390:LYS:HD2  | 6:N:743:HOH:O    | 2.10                     | 0.51              |
| 1:E:98:THR:O     | 1:E:102:GLY:CA   | 2.57                     | 0.51              |
| 1:C:161:ILE:HD13 | 1:C:196:VAL:HG21 | 1.90                     | 0.51              |
| 2:P:360:ASP:OD2  | 2:P:428:ARG:HD2  | 2.11                     | 0.51              |
| 2:M:416:LEU:C    | 2:M:416:LEU:HD23 | 2.36                     | 0.51              |
| 1:B:28:ASN:HB3   | 1:B:29:PRO:HD2   | 1.93                     | 0.51              |
| 1:E:62:LEU:HD13  | 1:E:101:ALA:O    | 2.11                     | 0.51              |
| 2:M:315:TRP:HZ2  | 2:M:503:GLN:NE2  | 2.07                     | 0.51              |
| 2:N:390:LYS:HD3  | 6:N:743:HOH:O    | 2.10                     | 0.51              |
| 1:A:191:GLY:O    | 1:A:194:GLU:HB2  | 2.10                     | 0.51              |
| 1:F:114:VAL:HG23 | 1:F:122:MET:HE2  | 1.92                     | 0.51              |
| 1:B:6:PRO:HB2    | 2:N:503:GLN:NE2  | 2.26                     | 0.50              |
| 1:C:33:GLN:OE1   | 2:O:355:GLY:N    | 2.34                     | 0.50              |
| 2:O:497:ASN:HD22 | 2:O:499:GLU:H    | 1.58                     | 0.50              |
| 2:M:434:ASP:HB3  | 2:M:436:TYR:CD2  | 2.47                     | 0.50              |
| 1:B:168:GLU:HA   | 1:B:171:ILE:HD12 | 1.93                     | 0.50              |
| 1:E:62:LEU:CD1   | 1:E:101:ALA:O    | 2.59                     | 0.50              |
| 1:F:48:HIS:C     | 1:F:180:LYS:HZ1  | 2.18                     | 0.50              |
| 2:N:361:HIS:ND1  | 4:N:601:BME:H21  | 2.26                     | 0.50              |
| 1:E:133:ARG:HG3  | 2:Q:326:THR:HG21 | 1.93                     | 0.50              |
| 1:F:19:ILE:O     | 2:R:426:VAL:HG21 | 2.12                     | 0.50              |
| 1:C:24:GLU:O     | 1:C:27:GLY:N     | 2.43                     | 0.50              |
| 1:C:98:THR:O     | 1:C:102:GLY:HA2  | 2.12                     | 0.50              |
| 1:D:163:GLN:HB3  | 1:D:165:GLN:NE2  | 2.27                     | 0.50              |
| 1:C:163:GLN:HB2  | 6:C:819:HOH:O    | 2.10                     | 0.50              |
| 2:R:434:ASP:HB3  | 2:R:436:TYR:CD2  | 2.47                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:116:ASN:C    | 1:C:116:ASN:OD1  | 2.53                     | 0.50              |
| 1:D:114:VAL:HG23 | 1:D:122:MET:CE   | 2.40                     | 0.50              |
| 2:P:400:TRP:HA   | 2:P:425:GLY:O    | 2.11                     | 0.50              |
| 2:R:473:LYS:HD2  | 2:R:474:LEU:N    | 2.26                     | 0.50              |
| 2:R:522:ARG:HE   | 2:R:524:ASP:CG   | 2.20                     | 0.50              |
| 1:B:140:HIS:O    | 1:B:197:PHE:HA   | 2.11                     | 0.50              |
| 2:Q:399:MET:HA   | 2:Q:462:HIS:O    | 2.11                     | 0.50              |
| 1:A:33:GLN:HB3   | 1:A:85:LEU:CD1   | 2.42                     | 0.49              |
| 1:E:31:ARG:HB2   | 1:E:34:GLU:OE2   | 2.11                     | 0.49              |
| 1:D:177:VAL:HG12 | 1:D:178:ASP:OD2  | 2.11                     | 0.49              |
| 2:P:437:TYR:CD1  | 2:P:437:TYR:C    | 2.91                     | 0.49              |
| 1:F:176:GLU:HA   | 1:F:180:LYS:O    | 2.11                     | 0.49              |
| 1:B:155:CYS:HB3  | 1:B:158:LEU:HB2  | 1.95                     | 0.49              |
| 2:R:383:ARG:HA   | 2:R:435:GLY:O    | 2.12                     | 0.49              |
| 1:A:160:LEU:HD12 | 2:M:339:ILE:HG22 | 1.93                     | 0.49              |
| 2:P:313:ARG:O    | 2:P:318:LYS:HE3  | 2.12                     | 0.49              |
| 1:E:50:LEU:O     | 1:E:182:ALA:HA   | 2.13                     | 0.49              |
| 1:F:36:TRP:CG    | 1:F:37:ASN:H     | 2.30                     | 0.49              |
| 1:F:48:HIS:C     | 1:F:180:LYS:HZ2  | 2.18                     | 0.49              |
| 2:M:376:GLU:O    | 2:M:442:ILE:HA   | 2.12                     | 0.49              |
| 1:C:36:TRP:CG    | 1:C:37:ASN:H     | 2.30                     | 0.49              |
| 2:R:432:ASP:OD1  | 2:R:434:ASP:N    | 2.45                     | 0.49              |
| 1:C:15:PRO:HB3   | 1:C:133:ARG:HD2  | 1.93                     | 0.49              |
| 2:O:326:THR:HG22 | 2:O:330:ARG:HD2  | 1.94                     | 0.49              |
| 1:D:65:ASP:OD2   | 1:D:133:ARG:HD3  | 2.12                     | 0.49              |
| 1:D:165:GLN:H    | 1:D:165:GLN:HE21 | 1.60                     | 0.49              |
| 2:P:325:LYS:HD3  | 2:Q:335:ALA:HB1  | 1.94                     | 0.49              |
| 1:E:84:ASN:HB3   | 1:E:87:ASN:ND2   | 2.28                     | 0.49              |
| 1:E:134:GLY:HA3  | 2:Q:326:THR:HG22 | 1.95                     | 0.49              |
| 1:A:110:LYS:NZ   | 1:A:147:ASP:OD1  | 2.41                     | 0.49              |
| 1:B:165:GLN:H    | 1:B:165:GLN:CD   | 2.05                     | 0.49              |
| 1:D:1:PRO:HG2    | 2:R:488:MET:HE2  | 1.95                     | 0.49              |
| 1:D:98:THR:O     | 1:D:102:GLY:HA2  | 2.12                     | 0.49              |
| 1:E:188:ARG:HG3  | 1:E:188:ARG:HH11 | 1.78                     | 0.49              |
| 1:E:190:GLN:NE2  | 2:Q:331:SER:O    | 2.35                     | 0.49              |
| 2:Q:404:ALA:HB2  | 2:Q:442:ILE:HD12 | 1.95                     | 0.49              |
| 2:R:437:TYR:CD1  | 2:R:437:TYR:C    | 2.91                     | 0.49              |
| 1:E:35:ILE:HG21  | 1:E:92:PHE:HE2   | 1.78                     | 0.48              |
| 1:F:176:GLU:OE2  | 1:F:179:GLY:HA2  | 2.13                     | 0.48              |
| 1:A:65:ASP:OD2   | 1:A:133:ARG:HD3  | 2.13                     | 0.48              |
| 1:F:23:LEU:HB2   | 1:F:30:THR:HG22  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:176:GLU:HA   | 1:C:180:LYS:O    | 2.13                     | 0.48              |
| 1:A:54:GLN:HG2   | 1:A:102:GLY:O    | 2.12                     | 0.48              |
| 1:C:70:VAL:HG11  | 1:C:106:LEU:HD21 | 1.95                     | 0.48              |
| 1:C:98:THR:C     | 1:C:100:ASP:H    | 2.20                     | 0.48              |
| 1:F:125:HIS:HA   | 1:F:143:LEU:O    | 2.14                     | 0.48              |
| 2:P:486:ILE:HB   | 2:P:487:PRO:HD3  | 1.94                     | 0.48              |
| 1:F:18:HIS:CE1   | 1:F:99:PHE:CE1   | 3.02                     | 0.48              |
| 1:F:188:ARG:HG3  | 1:F:188:ARG:NH1  | 2.25                     | 0.48              |
| 1:E:114:VAL:HG23 | 1:E:122:MET:CE   | 2.43                     | 0.48              |
| 2:R:385:VAL:O    | 2:R:526:VAL:HA   | 2.12                     | 0.48              |
| 2:M:373:PRO:HB3  | 2:M:423:PHE:HB2  | 1.95                     | 0.48              |
| 1:B:131:PHE:CE2  | 1:B:138:HIS:HB3  | 2.48                     | 0.48              |
| 2:P:489:CYS:HA   | 2:P:490:PRO:HD3  | 1.72                     | 0.48              |
| 1:E:161:ILE:HD13 | 1:E:196:VAL:HG21 | 1.95                     | 0.48              |
| 2:Q:478:LEU:C    | 2:Q:478:LEU:HD23 | 2.39                     | 0.48              |
| 2:R:350:ASN:OD1  | 2:R:352:SER:HB2  | 2.14                     | 0.48              |
| 1:F:131:PHE:CD2  | 2:R:475:ILE:HD12 | 2.49                     | 0.48              |
| 2:N:356:PHE:CD2  | 2:N:428:ARG:HD3  | 2.49                     | 0.48              |
| 1:C:35:ILE:HG21  | 1:C:92:PHE:CE2   | 2.48                     | 0.48              |
| 2:O:486:ILE:HB   | 2:O:487:PRO:HD3  | 1.95                     | 0.48              |
| 1:E:18:HIS:CE1   | 1:E:99:PHE:HE1   | 2.32                     | 0.48              |
| 1:E:143:LEU:HD23 | 1:E:143:LEU:C    | 2.39                     | 0.48              |
| 1:A:114:VAL:HG22 | 6:A:680:HOH:O    | 2.13                     | 0.47              |
| 1:D:131:PHE:CD2  | 1:D:138:HIS:HB3  | 2.49                     | 0.47              |
| 1:A:36:TRP:CG    | 1:A:37:ASN:H     | 2.33                     | 0.47              |
| 2:M:400:TRP:HA   | 2:M:425:GLY:O    | 2.14                     | 0.47              |
| 1:B:180:LYS:HD2  | 1:B:181:THR:N    | 2.29                     | 0.47              |
| 1:E:177:VAL:O    | 1:E:180:LYS:HB3  | 2.14                     | 0.47              |
| 1:B:36:TRP:CG    | 1:B:37:ASN:H     | 2.32                     | 0.47              |
| 1:C:98:THR:C     | 1:C:100:ASP:N    | 2.72                     | 0.47              |
| 2:O:416:LEU:HD23 | 2:O:417:ALA:N    | 2.29                     | 0.47              |
| 1:B:35:ILE:HG21  | 1:B:92:PHE:HE2   | 1.79                     | 0.47              |
| 1:C:131:PHE:CD2  | 1:C:138:HIS:HB3  | 2.49                     | 0.47              |
| 2:O:478:LEU:HD23 | 2:O:478:LEU:C    | 2.40                     | 0.47              |
| 1:D:165:GLN:H    | 1:D:165:GLN:CD   | 2.23                     | 0.47              |
| 2:Q:416:LEU:C    | 2:Q:416:LEU:CD2  | 2.87                     | 0.47              |
| 1:F:64:ARG:HH11  | 1:F:64:ARG:HD2   | 1.26                     | 0.47              |
| 1:A:70:VAL:HG21  | 1:A:106:LEU:HD21 | 1.97                     | 0.47              |
| 1:A:163:GLN:CB   | 1:A:165:GLN:HE22 | 2.28                     | 0.47              |
| 2:P:328:ILE:HD12 | 2:Q:335:ALA:HB2  | 1.97                     | 0.47              |
| 1:F:160:LEU:HD23 | 1:F:160:LEU:HA   | 1.77                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:437:TYR:CD1  | 2:M:437:TYR:C    | 2.92                     | 0.47              |
| 1:E:176:GLU:HA   | 1:E:180:LYS:O    | 2.14                     | 0.47              |
| 2:Q:406:GLY:O    | 2:Q:447:TYR:HD1  | 1.97                     | 0.47              |
| 1:F:35:ILE:HD13  | 2:R:351:PHE:CE1  | 2.50                     | 0.47              |
| 1:F:110:LYS:NZ   | 1:F:148:GLU:OE2  | 2.40                     | 0.47              |
| 1:F:116:ASN:OD1  | 1:F:116:ASN:C    | 2.57                     | 0.47              |
| 1:A:35:ILE:HD13  | 2:M:351:PHE:CE1  | 2.49                     | 0.46              |
| 1:B:49:ILE:HD12  | 1:B:51:LEU:HD21  | 1.95                     | 0.46              |
| 1:B:143:LEU:C    | 1:B:143:LEU:HD23 | 2.40                     | 0.46              |
| 1:C:58:GLY:HA3   | 1:C:190:GLN:OE1  | 2.15                     | 0.46              |
| 2:O:489:CYS:HA   | 2:O:490:PRO:HD3  | 1.66                     | 0.46              |
| 1:F:48:HIS:CD2   | 1:F:109:VAL:HG12 | 2.50                     | 0.46              |
| 1:A:16:TYR:O     | 1:A:19:ILE:HG23  | 2.15                     | 0.46              |
| 1:B:69:GLU:OE2   | 1:B:94:ARG:HD3   | 2.15                     | 0.46              |
| 2:O:437:TYR:OH   | 2:O:523:PHE:HB3  | 2.15                     | 0.46              |
| 2:P:434:ASP:HB3  | 2:P:436:TYR:CD2  | 2.50                     | 0.46              |
| 1:E:110:LYS:NZ   | 1:E:147:ASP:OD1  | 2.42                     | 0.46              |
| 1:F:41:LYS:HE3   | 1:F:85:LEU:O     | 2.15                     | 0.46              |
| 1:B:123:ALA:HB3  | 1:B:144:TYR:CE2  | 2.51                     | 0.46              |
| 1:E:22:ALA:O     | 1:E:25:ALA:HB3   | 2.15                     | 0.46              |
| 2:R:372:LEU:HD12 | 2:R:372:LEU:HA   | 1.69                     | 0.46              |
| 1:A:19:ILE:HG21  | 2:M:410:HIS:HB2  | 1.97                     | 0.46              |
| 1:C:19:ILE:HG12  | 2:O:400:TRP:HB2  | 1.97                     | 0.46              |
| 2:P:359:HIS:O    | 2:P:366:ASN:HB3  | 2.15                     | 0.46              |
| 1:C:131:PHE:O    | 1:C:132:ALA:CB   | 2.61                     | 0.46              |
| 2:Q:451:ASN:HB3  | 2:Q:455:ASP:OD2  | 2.16                     | 0.46              |
| 1:C:184:ARG:HG3  | 1:C:184:ARG:HH11 | 1.79                     | 0.46              |
| 1:E:116:ASN:OD1  | 1:E:116:ASN:C    | 2.59                     | 0.46              |
| 2:Q:497:ASN:HA   | 2:Q:498:PRO:HD2  | 1.70                     | 0.46              |
| 1:F:41:LYS:N     | 1:F:88:ALA:O     | 2.34                     | 0.46              |
| 1:A:50:LEU:O     | 1:A:182:ALA:HA   | 2.15                     | 0.46              |
| 2:N:489:CYS:HA   | 2:N:490:PRO:HD3  | 1.77                     | 0.46              |
| 2:O:356:PHE:HD1  | 2:O:428:ARG:HD3  | 1.78                     | 0.46              |
| 2:O:364:LEU:HD11 | 2:O:442:ILE:HG23 | 1.98                     | 0.46              |
| 1:A:131:PHE:CD2  | 1:A:138:HIS:HB3  | 2.51                     | 0.45              |
| 1:D:191:GLY:O    | 1:D:194:GLU:HB2  | 2.16                     | 0.45              |
| 2:Q:392:VAL:HG12 | 2:Q:395:THR:HB   | 1.98                     | 0.45              |
| 2:O:361:HIS:CD2  | 6:O:766:HOH:O    | 2.67                     | 0.45              |
| 2:Q:316:HIS:HB3  | 2:Q:317:PRO:HD2  | 1.99                     | 0.45              |
| 1:C:50:LEU:O     | 1:C:182:ALA:HA   | 2.16                     | 0.45              |
| 2:O:403:ASN:HB2  | 6:O:620:HOH:O    | 2.15                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:406:GLY:O    | 2:O:447:TYR:CD1  | 2.69                     | 0.45              |
| 1:D:36:TRP:CG    | 1:D:37:ASN:H     | 2.33                     | 0.45              |
| 2:R:497:ASN:HA   | 2:R:498:PRO:HD3  | 1.71                     | 0.45              |
| 1:F:3:GLU:OE1    | 1:F:3:GLU:HA     | 2.16                     | 0.45              |
| 2:R:392:VAL:HG12 | 2:R:395:THR:HB   | 1.98                     | 0.45              |
| 1:B:50:LEU:O     | 1:B:182:ALA:HA   | 2.17                     | 0.45              |
| 1:D:176:GLU:OE2  | 1:D:179:GLY:HA2  | 2.16                     | 0.45              |
| 1:F:37:ASN:HB2   | 1:F:106:LEU:HD12 | 1.97                     | 0.45              |
| 2:R:491:ILE:O    | 2:R:494:SER:OG   | 2.29                     | 0.45              |
| 1:C:64:ARG:HH11  | 1:C:64:ARG:HD2   | 1.55                     | 0.45              |
| 1:F:49:ILE:N     | 1:F:180:LYS:HZ1  | 2.15                     | 0.45              |
| 1:B:35:ILE:HG21  | 1:B:92:PHE:CE2   | 2.52                     | 0.45              |
| 1:C:3:GLU:OE1    | 1:C:3:GLU:HA     | 2.17                     | 0.45              |
| 2:O:390:LYS:CD   | 6:O:677:HOH:O    | 2.65                     | 0.45              |
| 1:E:51:LEU:HD11  | 1:E:126:ILE:HD12 | 1.99                     | 0.45              |
| 1:F:134:GLY:HA3  | 2:R:326:THR:HG22 | 1.99                     | 0.45              |
| 2:M:489:CYS:HA   | 2:M:490:PRO:HD3  | 1.72                     | 0.45              |
| 1:C:52:LEU:C     | 1:C:52:LEU:CD2   | 2.88                     | 0.45              |
| 1:C:176:GLU:HG3  | 1:C:180:LYS:C    | 2.41                     | 0.45              |
| 1:E:28:ASN:HB3   | 1:E:29:PRO:HD2   | 1.98                     | 0.45              |
| 2:Q:407:ARG:NH1  | 2:Q:417:ALA:O    | 2.46                     | 0.45              |
| 1:B:3:GLU:HA     | 1:B:3:GLU:OE1    | 2.17                     | 0.45              |
| 2:N:356:PHE:CE2  | 2:N:428:ARG:HD3  | 2.52                     | 0.45              |
| 1:C:160:LEU:HA   | 1:C:160:LEU:HD23 | 1.86                     | 0.45              |
| 2:P:335:ALA:HB1  | 2:R:325:LYS:HG2  | 1.98                     | 0.45              |
| 1:E:39:LEU:HD11  | 1:E:106:LEU:HD11 | 1.97                     | 0.45              |
| 2:Q:363:LEU:HD23 | 2:Q:425:GLY:HA2  | 1.99                     | 0.45              |
| 1:A:24:GLU:O     | 1:A:27:GLY:N     | 2.45                     | 0.44              |
| 2:O:497:ASN:HD22 | 2:O:498:PRO:CD   | 2.31                     | 0.44              |
| 1:D:19:ILE:CG2   | 2:P:410:HIS:HB2  | 2.46                     | 0.44              |
| 1:B:19:ILE:HD11  | 2:N:408:TYR:CD1  | 2.48                     | 0.44              |
| 1:D:154:LYS:HE3  | 1:D:154:LYS:N    | 2.32                     | 0.44              |
| 2:P:308:PHE:CE2  | 2:P:530:GLN:HB2  | 2.52                     | 0.44              |
| 2:P:335:ALA:HB2  | 2:R:328:ILE:HD12 | 1.99                     | 0.44              |
| 2:M:315:TRP:CZ2  | 2:M:503:GLN:NE2  | 2.82                     | 0.44              |
| 1:B:176:GLU:HG2  | 1:B:179:GLY:C    | 2.42                     | 0.44              |
| 2:N:414:ARG:HH11 | 2:N:414:ARG:HD2  | 1.49                     | 0.44              |
| 2:R:312:ASP:C    | 2:R:312:ASP:OD1  | 2.60                     | 0.44              |
| 1:A:31:ARG:NH1   | 2:M:428:ARG:HG2  | 2.33                     | 0.44              |
| 1:A:78:GLU:CG    | 2:M:301:PRO:CG   | 2.95                     | 0.44              |
| 1:D:19:ILE:HD11  | 2:P:408:TYR:CD2  | 2.44                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:497:ASN:HD22 | 2:P:497:ASN:C    | 2.26                     | 0.44              |
| 2:P:522:ARG:NH2  | 2:P:524:ASP:OD1  | 2.50                     | 0.44              |
| 1:E:52:LEU:O     | 1:E:184:ARG:HA   | 2.18                     | 0.44              |
| 2:Q:486:ILE:HB   | 2:Q:487:PRO:HD3  | 1.98                     | 0.44              |
| 1:B:176:GLU:HA   | 1:B:180:LYS:O    | 2.17                     | 0.44              |
| 2:O:497:ASN:HD22 | 2:O:498:PRO:N    | 2.16                     | 0.44              |
| 2:Q:497:ASN:ND2  | 2:Q:497:ASN:C    | 2.66                     | 0.44              |
| 2:N:364:LEU:HD12 | 2:N:373:PRO:HG2  | 1.99                     | 0.44              |
| 2:Q:383:ARG:HG3  | 2:Q:436:TYR:CE1  | 2.53                     | 0.44              |
| 2:R:306:SER:OG   | 2:R:530:GLN:NE2  | 2.35                     | 0.44              |
| 1:A:33:GLN:HB3   | 1:A:85:LEU:HD12  | 1.99                     | 0.44              |
| 2:R:399:MET:HE2  | 2:R:461:ILE:HG21 | 1.99                     | 0.44              |
| 1:A:99:PHE:HE2   | 2:M:411:LYS:HD2  | 1.83                     | 0.44              |
| 1:B:165:GLN:HE21 | 1:B:165:GLN:CA   | 2.30                     | 0.44              |
| 2:O:315:TRP:HZ2  | 2:O:503:GLN:HE21 | 1.66                     | 0.44              |
| 2:O:381:ALA:O    | 2:O:522:ARG:HA   | 2.18                     | 0.44              |
| 2:N:513:ALA:O    | 2:N:515:PRO:HD3  | 2.18                     | 0.44              |
| 2:P:356:PHE:CD1  | 2:P:428:ARG:HD3  | 2.53                     | 0.44              |
| 2:Q:383:ARG:N    | 2:Q:524:ASP:OD1  | 2.46                     | 0.44              |
| 2:M:341:GLN:HB3  | 2:M:346:THR:CG2  | 2.48                     | 0.43              |
| 1:B:80:GLN:O     | 1:B:91:SER:HB2   | 2.18                     | 0.43              |
| 1:E:120:VAL:HA   | 1:E:121:PRO:HD3  | 1.84                     | 0.43              |
| 2:M:310:ILE:CD1  | 2:O:453:PRO:HB2  | 2.45                     | 0.43              |
| 1:D:64:ARG:HH11  | 1:D:64:ARG:HD2   | 1.47                     | 0.43              |
| 2:P:376:GLU:OE1  | 6:P:677:HOH:O    | 2.20                     | 0.43              |
| 2:P:405:GLY:HA3  | 6:P:686:HOH:O    | 2.17                     | 0.43              |
| 2:Q:307:ARG:HG2  | 2:Q:533:THR:HG22 | 1.99                     | 0.43              |
| 2:R:432:ASP:OD1  | 2:R:432:ASP:C    | 2.61                     | 0.43              |
| 2:M:364:LEU:HB2  | 2:M:440:ARG:HD3  | 2.00                     | 0.43              |
| 2:O:393:PRO:O    | 2:O:393:PRO:HG2  | 2.17                     | 0.43              |
| 2:Q:390:LYS:HA   | 2:Q:391:PRO:HD3  | 1.84                     | 0.43              |
| 2:N:495:ILE:HG21 | 2:N:500:ALA:HB3  | 2.01                     | 0.43              |
| 1:D:176:GLU:HA   | 1:D:180:LYS:O    | 2.17                     | 0.43              |
| 1:E:58:GLY:CA    | 1:E:190:GLN:HB3  | 2.48                     | 0.43              |
| 1:E:84:ASN:HB3   | 1:E:87:ASN:CG    | 2.43                     | 0.43              |
| 1:E:131:PHE:O    | 1:E:132:ALA:HB2  | 2.18                     | 0.43              |
| 1:F:120:VAL:HA   | 1:F:121:PRO:HD3  | 1.82                     | 0.43              |
| 1:F:92:PHE:CG    | 2:R:349:PRO:HG3  | 2.54                     | 0.43              |
| 1:A:52:LEU:CD2   | 1:A:184:ARG:NH1  | 2.82                     | 0.43              |
| 1:C:114:VAL:HG23 | 1:C:122:MET:CE   | 2.44                     | 0.43              |
| 1:E:50:LEU:HD12  | 1:E:51:LEU:N     | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:100:ASP:OD1  | 1:E:100:ASP:N    | 2.52                     | 0.43              |
| 1:F:33:GLN:HG2   | 1:F:85:LEU:HD12  | 2.00                     | 0.43              |
| 2:Q:497:ASN:HD22 | 2:Q:499:GLU:H    | 1.66                     | 0.43              |
| 2:N:390:LYS:HA   | 2:N:391:PRO:HD3  | 1.83                     | 0.43              |
| 1:C:165:GLN:H    | 1:C:165:GLN:CD   | 2.26                     | 0.43              |
| 2:O:495:ILE:CG2  | 2:O:500:ALA:HB3  | 2.49                     | 0.43              |
| 1:E:174:ARG:HB2  | 1:E:183:TYR:CE1  | 2.53                     | 0.43              |
| 1:E:176:GLU:HG3  | 1:E:180:LYS:O    | 2.19                     | 0.43              |
| 1:F:20:GLY:HA2   | 2:R:426:VAL:HG13 | 2.01                     | 0.43              |
| 1:F:80:GLN:O     | 1:F:91:SER:HB2   | 2.19                     | 0.43              |
| 2:O:386:ASP:C    | 2:O:386:ASP:OD1  | 2.61                     | 0.43              |
| 2:O:497:ASN:HD22 | 2:O:498:PRO:HD2  | 1.84                     | 0.43              |
| 2:P:407:ARG:HD3  | 2:P:417:ALA:O    | 2.19                     | 0.43              |
| 2:P:495:ILE:CG2  | 2:P:500:ALA:HB3  | 2.48                     | 0.43              |
| 1:F:8:THR:HA     | 1:F:9:PRO:HD3    | 1.86                     | 0.43              |
| 2:R:505:ILE:O    | 2:R:507:LYS:HE3  | 2.19                     | 0.43              |
| 2:O:356:PHE:HD1  | 2:O:428:ARG:CD   | 2.31                     | 0.43              |
| 2:O:415:TYR:CE1  | 2:O:416:LEU:HD22 | 2.54                     | 0.43              |
| 2:Q:360:ASP:HB3  | 2:Q:428:ARG:HG3  | 2.01                     | 0.43              |
| 2:N:376:GLU:O    | 2:N:442:ILE:HA   | 2.18                     | 0.42              |
| 2:N:399:MET:HE2  | 2:N:461:ILE:HG21 | 2.01                     | 0.42              |
| 1:C:41:LYS:O     | 1:C:44:ALA:N     | 2.47                     | 0.42              |
| 1:C:184:ARG:NH1  | 1:C:184:ARG:HG3  | 2.34                     | 0.42              |
| 2:O:372:LEU:HA   | 2:O:373:PRO:HD3  | 1.84                     | 0.42              |
| 1:E:23:LEU:O     | 1:E:24:GLU:C     | 2.62                     | 0.42              |
| 1:A:44:ALA:O     | 1:A:48:HIS:NE2   | 2.40                     | 0.42              |
| 2:M:331:SER:HA   | 2:M:332:PRO:HD3  | 1.91                     | 0.42              |
| 2:M:484:PRO:O    | 2:M:487:PRO:HD2  | 2.19                     | 0.42              |
| 1:B:51:LEU:HD11  | 1:B:126:ILE:CD1  | 2.48                     | 0.42              |
| 1:C:28:ASN:HB3   | 6:C:807:HOH:O    | 2.18                     | 0.42              |
| 2:P:483:ASP:HA   | 2:P:484:PRO:HD2  | 1.87                     | 0.42              |
| 1:F:115:ASN:HA   | 1:F:121:PRO:HA   | 2.01                     | 0.42              |
| 2:R:372:LEU:HA   | 2:R:373:PRO:HD3  | 1.93                     | 0.42              |
| 2:M:385:VAL:O    | 2:M:526:VAL:HA   | 2.19                     | 0.42              |
| 1:C:70:VAL:HG21  | 1:C:106:LEU:HD21 | 2.02                     | 0.42              |
| 2:P:489:CYS:C    | 2:P:493:LYS:HE3  | 2.45                     | 0.42              |
| 1:E:8:THR:HA     | 1:E:9:PRO:HD3    | 1.87                     | 0.42              |
| 2:O:414:ARG:HH11 | 2:O:414:ARG:HD2  | 1.63                     | 0.42              |
| 1:A:1:PRO:HG2    | 2:O:488:MET:HE2  | 2.00                     | 0.42              |
| 1:A:15:PRO:HB3   | 1:A:133:ARG:HD2  | 2.01                     | 0.42              |
| 1:A:74:ASP:OD1   | 1:A:74:ASP:C     | 2.63                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:473:LYS:NZ   | 6:P:691:HOH:O    | 2.50                     | 0.42              |
| 2:R:415:TYR:CE1  | 2:R:416:LEU:HD22 | 2.52                     | 0.42              |
| 2:R:460:HIS:HA   | 2:R:478:LEU:O    | 2.19                     | 0.42              |
| 1:D:51:LEU:CD1   | 1:D:126:ILE:HD12 | 2.49                     | 0.42              |
| 1:D:72:GLN:O     | 1:D:91:SER:OG    | 2.37                     | 0.42              |
| 1:F:35:ILE:CD1   | 2:R:351:PHE:CE1  | 3.03                     | 0.42              |
| 1:A:64:ARG:NE    | 1:A:100:ASP:O    | 2.49                     | 0.42              |
| 1:C:31:ARG:NH1   | 2:O:428:ARG:HG2  | 2.35                     | 0.42              |
| 1:C:140:HIS:O    | 1:C:197:PHE:HA   | 2.19                     | 0.42              |
| 2:P:399:MET:HA   | 2:P:462:HIS:O    | 2.20                     | 0.42              |
| 2:N:488:MET:CE   | 1:C:1:PRO:HG2    | 2.49                     | 0.42              |
| 1:C:70:VAL:HG11  | 1:C:106:LEU:CD2  | 2.50                     | 0.42              |
| 1:D:51:LEU:HD11  | 1:D:126:ILE:CD1  | 2.48                     | 0.42              |
| 2:Q:420:ASP:HA   | 2:Q:421:PRO:HD2  | 1.78                     | 0.42              |
| 2:M:376:GLU:HG2  | 2:P:446:PRO:HD2  | 2.01                     | 0.42              |
| 1:C:161:ILE:CD1  | 1:C:196:VAL:HG11 | 2.50                     | 0.42              |
| 2:O:497:ASN:HA   | 2:O:498:PRO:HD2  | 1.93                     | 0.42              |
| 2:P:522:ARG:NH1  | 6:P:704:HOH:O    | 2.50                     | 0.42              |
| 2:Q:302:ALA:HB1  | 2:Q:347:THR:CG2  | 2.50                     | 0.42              |
| 2:R:390:LYS:HA   | 2:R:391:PRO:HD3  | 1.87                     | 0.42              |
| 2:M:359:HIS:O    | 2:M:366:ASN:HB3  | 2.20                     | 0.41              |
| 1:C:28:ASN:HB3   | 1:C:29:PRO:HD2   | 2.01                     | 0.41              |
| 1:C:123:ALA:HA   | 1:C:124:PRO:HD3  | 1.94                     | 0.41              |
| 2:P:313:ARG:O    | 2:P:318:LYS:CE   | 2.68                     | 0.41              |
| 1:E:36:TRP:CG    | 1:E:37:ASN:H     | 2.37                     | 0.41              |
| 2:Q:489:CYS:HA   | 2:Q:490:PRO:HD3  | 1.87                     | 0.41              |
| 2:R:450:ARG:HH11 | 2:R:450:ARG:HD2  | 1.55                     | 0.41              |
| 1:A:165:GLN:NE2  | 1:A:165:GLN:H    | 2.17                     | 0.41              |
| 1:E:39:LEU:HD11  | 1:E:93:GLY:HA3   | 2.02                     | 0.41              |
| 1:F:74:ASP:HB3   | 1:F:89:PHE:CD2   | 2.55                     | 0.41              |
| 1:F:122:MET:HE3  | 1:F:125:HIS:HE1  | 1.85                     | 0.41              |
| 2:R:305:ASN:N    | 6:R:879:HOH:O    | 2.35                     | 0.41              |
| 2:R:513:ALA:O    | 2:R:515:PRO:HD3  | 2.20                     | 0.41              |
| 1:A:110:LYS:HE2  | 1:A:148:GLU:OE2  | 2.20                     | 0.41              |
| 2:N:324:TYR:OH   | 5:N:550:INO:O1   | 2.30                     | 0.41              |
| 2:N:495:ILE:CG2  | 2:N:500:ALA:HB3  | 2.49                     | 0.41              |
| 2:N:536:GLU:HB2  | 6:N:799:HOH:O    | 2.20                     | 0.41              |
| 1:C:164:PRO:HA   | 1:C:167:ARG:HD2  | 2.02                     | 0.41              |
| 1:E:92:PHE:CG    | 2:Q:349:PRO:HG3  | 2.55                     | 0.41              |
| 1:E:165:GLN:NE2  | 1:E:165:GLN:N    | 2.21                     | 0.41              |
| 2:Q:488:MET:HE2  | 1:F:1:PRO:HG2    | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:64:ARG:NE    | 1:B:100:ASP:O    | 2.45                     | 0.41              |
| 2:O:410:HIS:ND1  | 2:O:411:LYS:N    | 2.68                     | 0.41              |
| 1:D:39:LEU:HD11  | 1:D:93:GLY:HA3   | 2.01                     | 0.41              |
| 2:P:495:ILE:HG21 | 2:P:500:ALA:HB3  | 2.01                     | 0.41              |
| 2:Q:312:ASP:OD1  | 2:Q:312:ASP:C    | 2.63                     | 0.41              |
| 2:R:495:ILE:CG2  | 2:R:500:ALA:HB3  | 2.50                     | 0.41              |
| 2:M:356:PHE:HD1  | 2:M:428:ARG:HD3  | 1.86                     | 0.41              |
| 1:F:53:GLY:HA3   | 1:F:185:PHE:O    | 2.20                     | 0.41              |
| 2:M:508:LEU:CD2  | 2:P:488:MET:HE1  | 2.41                     | 0.41              |
| 1:B:35:ILE:HD13  | 2:N:351:PHE:CE1  | 2.56                     | 0.41              |
| 2:N:331:SER:HA   | 2:N:332:PRO:HD3  | 1.88                     | 0.41              |
| 2:P:416:LEU:C    | 2:P:416:LEU:CD2  | 2.92                     | 0.41              |
| 1:F:110:LYS:HE2  | 1:F:148:GLU:OE2  | 2.21                     | 0.41              |
| 1:F:190:GLN:NE2  | 2:R:331:SER:O    | 2.32                     | 0.41              |
| 2:O:392:VAL:HG12 | 2:O:395:THR:HB   | 2.02                     | 0.41              |
| 1:D:52:LEU:CD2   | 1:D:184:ARG:NH1  | 2.84                     | 0.41              |
| 1:F:19:ILE:O     | 2:R:426:VAL:CG2  | 2.68                     | 0.41              |
| 2:M:362:ASP:CG   | 2:M:440:ARG:HD2  | 2.46                     | 0.41              |
| 2:M:434:ASP:HB3  | 2:M:436:TYR:CE2  | 2.56                     | 0.41              |
| 2:M:519:LEU:HD23 | 2:M:519:LEU:HA   | 1.94                     | 0.41              |
| 2:N:497:ASN:HA   | 2:N:498:PRO:HD3  | 1.87                     | 0.41              |
| 1:C:19:ILE:HG21  | 1:C:19:ILE:HD13  | 1.81                     | 0.41              |
| 1:C:39:LEU:O     | 1:C:89:PHE:HA    | 2.21                     | 0.41              |
| 2:O:516:MET:HE3  | 2:O:516:MET:HB3  | 1.82                     | 0.41              |
| 1:D:98:THR:OG1   | 1:D:102:GLY:N    | 2.51                     | 0.41              |
| 2:P:364:LEU:HB2  | 2:P:440:ARG:HD3  | 2.02                     | 0.41              |
| 1:E:4:LEU:HB3    | 2:Q:387:GLN:HB3  | 2.03                     | 0.41              |
| 1:E:194:GLU:OE2  | 2:Q:334:GLN:HB2  | 2.21                     | 0.41              |
| 1:F:48:HIS:CD2   | 1:F:48:HIS:N     | 2.88                     | 0.41              |
| 2:R:307:ARG:NE   | 2:R:536:GLU:OE2  | 2.51                     | 0.41              |
| 1:A:61:HIS:ND1   | 1:B:163:GLN:HG3  | 2.36                     | 0.41              |
| 1:B:8:THR:HA     | 1:B:9:PRO:HD3    | 1.95                     | 0.41              |
| 1:B:39:LEU:HD11  | 1:B:93:GLY:HA3   | 2.03                     | 0.41              |
| 1:C:19:ILE:HG13  | 2:O:426:VAL:HG22 | 2.03                     | 0.41              |
| 1:E:58:GLY:HA2   | 1:E:190:GLN:HB3  | 2.02                     | 0.41              |
| 2:N:315:TRP:HZ2  | 2:N:503:GLN:NE2  | 2.17                     | 0.40              |
| 2:O:331:SER:HA   | 2:O:332:PRO:HD3  | 1.94                     | 0.40              |
| 2:O:437:TYR:CD1  | 2:O:437:TYR:C    | 2.99                     | 0.40              |
| 1:A:198:PHE:HA   | 2:M:337:VAL:O    | 2.20                     | 0.40              |
| 2:N:516:MET:HE3  | 2:N:516:MET:HB3  | 1.85                     | 0.40              |
| 1:D:143:LEU:C    | 1:D:143:LEU:HD23 | 2.46                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:Q:360:ASP:OD2 | 2:Q:428:ARG:HD2  | 2.22                     | 0.40              |
| 2:R:444:PRO:O   | 2:R:459:ALA:HB1  | 2.20                     | 0.40              |
| 1:A:78:GLU:HG3  | 2:M:301:PRO:HG3  | 2.04                     | 0.40              |
| 2:M:406:GLY:O   | 2:M:447:TYR:HD1  | 2.03                     | 0.40              |
| 1:D:131:PHE:CE2 | 1:D:138:HIS:HB3  | 2.56                     | 0.40              |
| 1:D:133:ARG:HG3 | 2:P:326:THR:HG21 | 2.04                     | 0.40              |
| 1:E:188:ARG:CG  | 1:E:188:ARG:NH1  | 2.83                     | 0.40              |
| 2:R:443:LYS:HE2 | 2:R:480:PHE:CG   | 2.56                     | 0.40              |
| 1:A:41:LYS:HB2  | 1:A:88:ALA:HA    | 2.04                     | 0.40              |
| 1:B:74:ASP:HB2  | 6:B:690:HOH:O    | 2.21                     | 0.40              |
| 1:B:145:PHE:CD1 | 1:B:145:PHE:N    | 2.89                     | 0.40              |
| 1:A:78:GLU:HG2  | 2:M:301:PRO:HB3  | 2.00                     | 0.40              |
| 1:C:19:ILE:CG1  | 2:O:400:TRP:HB2  | 2.52                     | 0.40              |
| 2:O:356:PHE:CD1 | 2:O:428:ARG:CD   | 3.04                     | 0.40              |
| 2:O:362:ASP:OD1 | 2:O:440:ARG:HD3  | 2.21                     | 0.40              |
| 1:F:176:GLU:HG3 | 1:F:180:LYS:H    | 1.85                     | 0.40              |
| 2:R:516:MET:HE3 | 2:R:516:MET:HB3  | 1.84                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 198/200 (99%) | 188 (95%) | 10 (5%) | 0        | 100         | 100 |
| 1   | B     | 198/200 (99%) | 188 (95%) | 10 (5%) | 0        | 100         | 100 |
| 1   | C     | 198/200 (99%) | 189 (96%) | 8 (4%)  | 1 (0%)   | 24          | 19  |
| 1   | D     | 198/200 (99%) | 187 (94%) | 11 (6%) | 0        | 100         | 100 |
| 1   | E     | 198/200 (99%) | 187 (94%) | 11 (6%) | 0        | 100         | 100 |
| 1   | F     | 198/200 (99%) | 188 (95%) | 9 (4%)  | 1 (0%)   | 24          | 19  |
| 2   | M     | 229/238 (96%) | 219 (96%) | 10 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2   | N     | 229/238 (96%)   | 221 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 2   | O     | 229/238 (96%)   | 222 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 2   | P     | 229/238 (96%)   | 224 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 2   | Q     | 229/238 (96%)   | 221 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 2   | R     | 229/238 (96%)   | 222 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| All | All   | 2562/2628 (98%) | 2456 (96%) | 104 (4%) | 2 (0%)   | 48          | 49  |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 101 | ALA  |
| 1   | F     | 74  | ASP  |

### 5.3.2 Protein sidechains [i](#)

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%)   | 153 (94%)  | 9 (6%)   | 19          | 14 |
| 1   | B     | 162/163 (99%)   | 151 (93%)  | 11 (7%)  | 14          | 9  |
| 1   | C     | 162/163 (99%)   | 155 (96%)  | 7 (4%)   | 26          | 23 |
| 1   | D     | 162/163 (99%)   | 155 (96%)  | 7 (4%)   | 26          | 23 |
| 1   | E     | 162/163 (99%)   | 154 (95%)  | 8 (5%)   | 22          | 18 |
| 1   | F     | 162/163 (99%)   | 155 (96%)  | 7 (4%)   | 26          | 23 |
| 2   | M     | 196/202 (97%)   | 182 (93%)  | 14 (7%)  | 13          | 8  |
| 2   | N     | 196/202 (97%)   | 189 (96%)  | 7 (4%)   | 31          | 30 |
| 2   | O     | 196/202 (97%)   | 184 (94%)  | 12 (6%)  | 17          | 12 |
| 2   | P     | 196/202 (97%)   | 186 (95%)  | 10 (5%)  | 21          | 17 |
| 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%) | 2036 (95%) | 112 (5%) | 21          | 16 |

All (112) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | LEU  |
| 1   | A     | 19  | ILE  |
| 1   | A     | 38  | ARG  |
| 1   | A     | 42  | PRO  |
| 1   | A     | 52  | LEU  |
| 1   | A     | 100 | ASP  |
| 1   | A     | 143 | LEU  |
| 1   | A     | 165 | GLN  |
| 1   | A     | 188 | ARG  |
| 2   | M     | 301 | PRO  |
| 2   | M     | 326 | THR  |
| 2   | M     | 364 | LEU  |
| 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     | 442 | ILE  |
| 2   | M     | 488 | MET  |
| 2   | M     | 497 | ASN  |
| 2   | M     | 507 | LYS  |
| 2   | M     | 534 | HIS  |
| 1   | B     | 4   | LEU  |
| 1   | B     | 19  | ILE  |
| 1   | B     | 42  | PRO  |
| 1   | B     | 52  | LEU  |
| 1   | B     | 64  | ARG  |
| 1   | B     | 100 | ASP  |
| 1   | B     | 106 | LEU  |
| 1   | B     | 154 | LYS  |
| 1   | B     | 158 | LEU  |
| 1   | B     | 165 | GLN  |
| 1   | B     | 176 | GLU  |
| 2   | N     | 364 | LEU  |
| 2   | N     | 372 | LEU  |
| 2   | N     | 395 | THR  |
| 2   | N     | 416 | LEU  |
| 2   | N     | 478 | LEU  |
| 2   | N     | 497 | ASN  |
| 2   | N     | 507 | LYS  |
| 1   | C     | 4   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 19  | ILE  |
| 1   | C     | 38  | ARG  |
| 1   | C     | 52  | LEU  |
| 1   | C     | 100 | ASP  |
| 1   | C     | 154 | LYS  |
| 1   | C     | 165 | GLN  |
| 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     | 428 | ARG  |
| 2   | O     | 433 | SER  |
| 2   | O     | 434 | ASP  |
| 2   | O     | 442 | ILE  |
| 2   | O     | 478 | LEU  |
| 2   | O     | 507 | LYS  |
| 1   | D     | 4   | LEU  |
| 1   | D     | 19  | ILE  |
| 1   | D     | 52  | LEU  |
| 1   | D     | 100 | ASP  |
| 1   | D     | 154 | LYS  |
| 1   | D     | 165 | GLN  |
| 1   | D     | 180 | LYS  |
| 2   | P     | 372 | LEU  |
| 2   | P     | 395 | THR  |
| 2   | P     | 411 | LYS  |
| 2   | P     | 416 | LEU  |
| 2   | P     | 434 | ASP  |
| 2   | P     | 442 | ILE  |
| 2   | P     | 478 | LEU  |
| 2   | P     | 497 | ASN  |
| 2   | P     | 503 | GLN  |
| 2   | P     | 534 | HIS  |
| 1   | E     | 4   | LEU  |
| 1   | E     | 19  | ILE  |
| 1   | E     | 52  | LEU  |
| 1   | E     | 100 | ASP  |
| 1   | E     | 165 | GLN  |
| 1   | E     | 178 | ASP  |
| 1   | E     | 180 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 181 | THR  |
| 2   | Q     | 364 | LEU  |
| 2   | Q     | 372 | LEU  |
| 2   | Q     | 395 | THR  |
| 2   | Q     | 416 | LEU  |
| 2   | Q     | 428 | ARG  |
| 2   | Q     | 438 | SER  |
| 2   | Q     | 475 | ILE  |
| 2   | Q     | 478 | LEU  |
| 2   | Q     | 497 | ASN  |
| 2   | Q     | 507 | LYS  |
| 1   | F     | 4   | LEU  |
| 1   | F     | 19  | ILE  |
| 1   | F     | 52  | LEU  |
| 1   | F     | 100 | ASP  |
| 1   | F     | 165 | GLN  |
| 1   | F     | 176 | GLU  |
| 1   | F     | 181 | THR  |
| 2   | R     | 310 | ILE  |
| 2   | R     | 372 | LEU  |
| 2   | R     | 395 | THR  |
| 2   | R     | 416 | LEU  |
| 2   | R     | 428 | ARG  |
| 2   | R     | 434 | ASP  |
| 2   | R     | 473 | LYS  |
| 2   | R     | 478 | LEU  |
| 2   | R     | 497 | ASN  |
| 2   | R     | 507 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | HIS  |
| 1   | A     | 84  | ASN  |
| 1   | A     | 87  | ASN  |
| 1   | A     | 165 | GLN  |
| 2   | M     | 359 | HIS  |
| 2   | M     | 361 | HIS  |
| 2   | M     | 412 | ASN  |
| 2   | M     | 497 | ASN  |
| 2   | M     | 503 | GLN  |
| 1   | B     | 140 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 165 | GLN  |
| 2   | N     | 361 | HIS  |
| 2   | N     | 412 | ASN  |
| 2   | N     | 497 | ASN  |
| 2   | N     | 503 | GLN  |
| 2   | N     | 534 | HIS  |
| 1   | C     | 11  | GLN  |
| 1   | C     | 18  | HIS  |
| 1   | C     | 87  | ASN  |
| 1   | C     | 163 | GLN  |
| 1   | C     | 165 | GLN  |
| 2   | O     | 361 | HIS  |
| 2   | O     | 497 | ASN  |
| 2   | O     | 503 | GLN  |
| 1   | D     | 18  | HIS  |
| 1   | D     | 163 | GLN  |
| 1   | D     | 165 | GLN  |
| 2   | P     | 305 | ASN  |
| 2   | P     | 334 | GLN  |
| 2   | P     | 361 | HIS  |
| 2   | P     | 412 | ASN  |
| 2   | P     | 497 | ASN  |
| 2   | P     | 503 | GLN  |
| 2   | P     | 530 | GLN  |
| 1   | E     | 11  | GLN  |
| 1   | E     | 18  | HIS  |
| 1   | E     | 165 | GLN  |
| 2   | Q     | 361 | HIS  |
| 2   | Q     | 497 | ASN  |
| 2   | Q     | 503 | GLN  |
| 2   | Q     | 512 | ASN  |
| 2   | Q     | 530 | GLN  |
| 2   | Q     | 534 | HIS  |
| 1   | F     | 11  | GLN  |
| 1   | F     | 54  | GLN  |
| 1   | F     | 59  | ASN  |
| 1   | F     | 115 | ASN  |
| 1   | F     | 165 | GLN  |
| 2   | R     | 359 | HIS  |
| 2   | R     | 361 | HIS  |
| 2   | R     | 497 | ASN  |
| 2   | R     | 503 | GLN  |

### 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  | M     | 601 | 2    | 3,3,3        | 0.68 | 0           | 2,2,2       | 1.04 | 0           |
| 5   | INO  | Q     | 550 | 3    | 10,11,11     | 1.81 | 4 (40%)     | 10,15,15    | 0.99 | 1 (10%)     |
| 5   | INO  | R     | 550 | 3    | 10,11,11     | 1.90 | 3 (30%)     | 10,15,15    | 0.98 | 1 (10%)     |
| 4   | BME  | Q     | 601 | 2    | 3,3,3        | 0.97 | 0           | 2,2,2       | 1.06 | 0           |
| 4   | BME  | N     | 601 | 2    | 3,3,3        | 0.62 | 0           | 2,2,2       | 1.31 | 0           |
| 4   | BME  | O     | 601 | 2    | 3,3,3        | 0.54 | 0           | 2,2,2       | 0.73 | 0           |
| 5   | INO  | M     | 550 | 3    | 10,11,11     | 1.91 | 4 (40%)     | 10,15,15    | 1.27 | 2 (20%)     |
| 5   | INO  | P     | 550 | 3    | 10,11,11     | 1.76 | 3 (30%)     | 10,15,15    | 1.07 | 1 (10%)     |
| 4   | BME  | R     | 601 | 2    | 3,3,3        | 0.41 | 0           | 2,2,2       | 0.71 | 0           |
| 5   | INO  | N     | 550 | 3    | 10,11,11     | 1.86 | 4 (40%)     | 10,15,15    | 1.07 | 1 (10%)     |
| 4   | BME  | P     | 601 | 2    | 3,3,3        | 0.79 | 0           | 2,2,2       | 1.63 | 1 (50%)     |
| 5   | INO  | O     | 550 | 3    | 10,11,11     | 1.73 | 3 (30%)     | 10,15,15    | 0.98 | 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  | M     | 601 | 2    | -       | 0/1/1/1  | -       |
| 5   | INO  | Q     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 5   | INO  | R     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 4   | BME  | Q     | 601 | 2    | -       | 1/1/1/1  | -       |
| 4   | BME  | N     | 601 | 2    | -       | 1/1/1/1  | -       |
| 4   | BME  | O     | 601 | 2    | -       | 0/1/1/1  | -       |
| 5   | INO  | M     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 5   | INO  | P     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 4   | BME  | R     | 601 | 2    | -       | 1/1/1/1  | -       |
| 5   | INO  | N     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |
| 4   | BME  | P     | 601 | 2    | -       | 0/1/1/1  | -       |
| 5   | INO  | O     | 550 | 3    | -       | 0/4/4/4  | 0/1/1/1 |

All (21) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | R     | 550 | INO  | O3-C2 | -3.45 | 1.23        | 1.32     |
| 5   | N     | 550 | INO  | O3-C2 | -3.28 | 1.23        | 1.32     |
| 5   | M     | 550 | INO  | O3-C2 | -3.21 | 1.24        | 1.32     |
| 5   | P     | 550 | INO  | O3-C2 | -3.11 | 1.24        | 1.32     |
| 5   | Q     | 550 | INO  | C3-C4 | 2.91  | 1.43        | 1.39     |
| 5   | N     | 550 | INO  | O4-N1 | -2.91 | 1.31        | 1.37     |
| 5   | O     | 550 | INO  | O3-C2 | -2.57 | 1.25        | 1.32     |
| 5   | O     | 550 | INO  | C3-C4 | 2.55  | 1.43        | 1.39     |
| 5   | P     | 550 | INO  | C4-C7 | 2.54  | 1.54        | 1.49     |
| 5   | Q     | 550 | INO  | O3-C2 | -2.54 | 1.25        | 1.32     |
| 5   | R     | 550 | INO  | O4-N1 | -2.50 | 1.32        | 1.37     |
| 5   | M     | 550 | INO  | C4-C7 | 2.47  | 1.54        | 1.49     |
| 5   | O     | 550 | INO  | C4-C7 | 2.33  | 1.54        | 1.49     |
| 5   | M     | 550 | INO  | O2-C7 | -2.31 | 1.23        | 1.30     |
| 5   | N     | 550 | INO  | O2-C7 | -2.27 | 1.23        | 1.30     |
| 5   | M     | 550 | INO  | O4-N1 | -2.26 | 1.32        | 1.37     |
| 5   | Q     | 550 | INO  | C4-C7 | 2.12  | 1.54        | 1.49     |
| 5   | P     | 550 | INO  | C2-N1 | -2.11 | 1.31        | 1.35     |
| 5   | Q     | 550 | INO  | C2-N1 | -2.11 | 1.31        | 1.35     |
| 5   | R     | 550 | INO  | C2-N1 | -2.09 | 1.31        | 1.35     |
| 5   | N     | 550 | INO  | C4-C7 | 2.04  | 1.53        | 1.49     |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | M     | 550 | INO  | O2-C7-C4 | 2.69  | 121.73      | 114.84   |
| 4   | P     | 601 | BME  | O1-C1-C2 | -2.30 | 101.85      | 110.82   |
| 5   | R     | 550 | INO  | O2-C7-O1 | -2.16 | 118.72      | 123.35   |
| 5   | M     | 550 | INO  | O2-C7-O1 | -2.12 | 118.80      | 123.35   |
| 5   | Q     | 550 | INO  | O2-C7-C4 | 2.09  | 120.20      | 114.84   |
| 5   | N     | 550 | INO  | O2-C7-O1 | -2.05 | 118.94      | 123.35   |
| 5   | P     | 550 | INO  | O2-C7-C4 | 2.01  | 119.99      | 114.84   |

There are no chirality outliers.

All (3) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | N     | 601 | BME  | O1-C1-C2-S2 |
| 4   | Q     | 601 | BME  | O1-C1-C2-S2 |
| 4   | R     | 601 | BME  | O1-C1-C2-S2 |

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | N     | 601 | BME  | 1       | 0            |
| 5   | N     | 550 | INO  | 1       | 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.