



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:38 PM UTC

PDB ID : 2Z8Y / pdb\_00002z8y  
Title : Xenon-bound structure of bifunctional carbon monoxide dehydrogenase/acet  
yl-CoA synthase(CODH/ACS) from Moorella thermoacetica  
Authors : Doukov, T.I.; Blasiak, L.C.; Drennan, C.L.  
Deposited on : 2007-09-12  
Resolution : 2.51 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) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

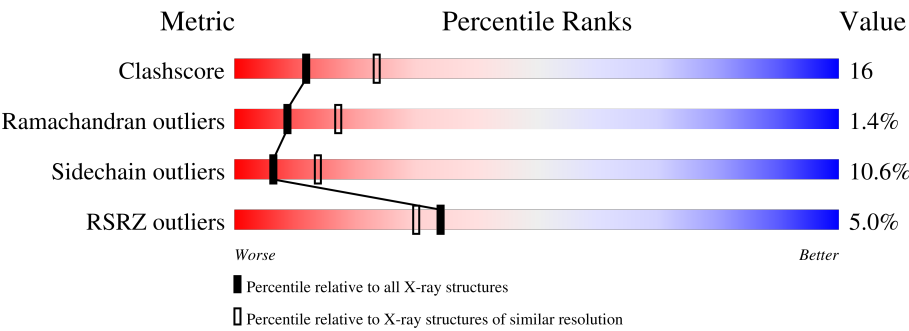
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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                      | 6492 (2.50-2.50)                                      |
| Ramachandran outliers | 187476                      | 6378 (2.50-2.50)                                      |
| Sidechain outliers    | 187428                      | 6380 (2.50-2.50)                                      |
| RSRZ outliers         | 180081                      | 5833 (2.50-2.50)                                      |

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                 |
|-----|-------|--------|--------------------------------------------------|
| 1   | A     | 674    | <div><div></div><div>70%26%.</div></div>         |
| 1   | B     | 674    | <div><div></div><div>70%25%.</div></div>         |
| 1   | C     | 674    | <div><div></div><div>70%25%.</div></div>         |
| 1   | D     | 674    | <div><div></div><div>64%32%.</div></div>         |
| 2   | M     | 729    | <div><div>%</div><div>70%24%5%.</div></div>      |
| 2   | N     | 729    | <div><div></div><div>68%27%. .</div></div>       |
| 2   | O     | 729    | <div><div>24%</div><div>41%41%16%. .</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | P     | 729    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res     | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|---------|-----------|----------|---------|------------------|
| 3   | SF4  | O     | 900     | -         | -        | X       | -                |
| 4   | XCC  | A     | 800     | -         | -        | X       | -                |
| 4   | XCC  | B     | 800     | -         | -        | X       | -                |
| 4   | XCC  | C     | 800     | -         | -        | X       | -                |
| 5   | XE   | A     | 1001    | -         | -        | X       | -                |
| 5   | XE   | A     | 1003[A] | -         | -        | X       | -                |
| 5   | XE   | A     | 1003[B] | -         | -        | X       | -                |
| 5   | XE   | A     | 1004    | -         | -        | X       | -                |
| 5   | XE   | B     | 1001    | -         | -        | X       | -                |
| 5   | XE   | B     | 1003[B] | -         | -        | X       | -                |
| 5   | XE   | B     | 1004    | -         | -        | X       | -                |
| 5   | XE   | C     | 1003[B] | -         | -        | X       | -                |
| 5   | XE   | C     | 1004    | -         | -        | X       | -                |
| 5   | XE   | D     | 1003[B] | -         | -        | X       | -                |
| 5   | XE   | M     | 1006    | -         | -        | X       | -                |
| 5   | XE   | N     | 1006    | -         | -        | X       | -                |
| 5   | XE   | N     | 1009    | -         | -        | X       | -                |
| 5   | XE   | O     | 1006    | -         | -        | X       | -                |
| 5   | XE   | O     | 1009    | -         | -        | X       | -                |
| 5   | XE   | P     | 1008    | -         | -        | X       | -                |
| 6   | GOL  | A     | 862     | -         | -        | X       | -                |
| 6   | GOL  | D     | 863     | -         | -        | X       | -                |

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 44706 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 Carbon monoxide dehydrogenase/acetyl CoA synthase subunit beta.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 673      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 5094  | 3202 | 891 | 959 | 42 |         |         |       |
| 1   | B     | 673      | Total | C    | N   | O   | S  | 0       | 7       | 0     |
|     |       |          | 5094  | 3202 | 891 | 959 | 42 |         |         |       |
| 1   | C     | 673      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 5094  | 3202 | 891 | 959 | 42 |         |         |       |
| 1   | D     | 673      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 5094  | 3202 | 891 | 959 | 42 |         |         |       |

- Molecule 2 is a protein called Carbon monoxide dehydrogenase/acetyl CoA synthase subunit alpha.

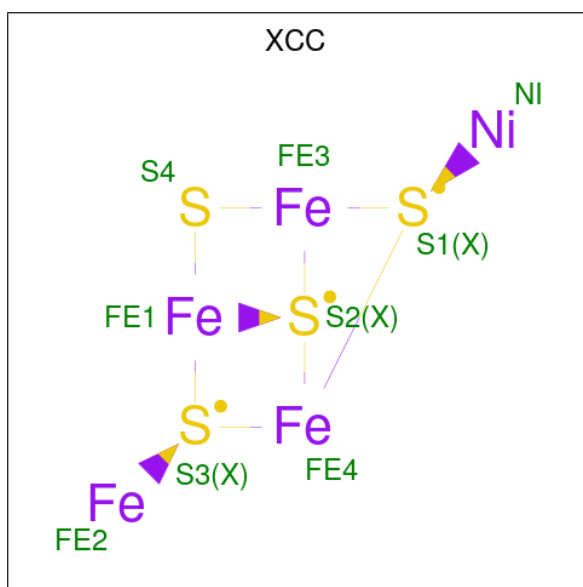
| Mol | Chain | Residues | Atoms |      |     |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|---------|-------|
| 2   | M     | 728      | Total | C    | N   | O    | S  | 0       | 4       | 0     |
|     |       |          | 5740  | 3681 | 956 | 1068 | 35 |         |         |       |
| 2   | N     | 728      | Total | C    | N   | O    | S  | 0       | 3       | 0     |
|     |       |          | 5740  | 3681 | 956 | 1068 | 35 |         |         |       |
| 2   | O     | 727      | Total | C    | N   | O    | S  | 0       | 1       | 0     |
|     |       |          | 5725  | 3673 | 952 | 1066 | 34 |         |         |       |
| 2   | P     | 728      | Total | C    | N   | O    | S  | 0       | 3       | 0     |
|     |       |          | 5740  | 3681 | 956 | 1068 | 35 |         |         |       |

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 3   | A     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 3   | A     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 3   | B     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 3   | C     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 3   | C     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 3   | D     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 3   | M     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 3   | N     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 3   | O     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 3   | P     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

- Molecule 4 is FE(4)-NI(1)-S(4) CLUSTER (CCD ID: XCC) (formula: Fe<sub>4</sub>NiS<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 4   | A     | 1        | Total | Fe | Ni | S | 0       | 0       |
|     |       |          | 9     | 4  | 1  | 4 |         |         |
| 4   | B     | 1        | Total | Fe | Ni | S | 0       | 0       |
|     |       |          | 9     | 4  | 1  | 4 |         |         |
| 4   | C     | 1        | Total | Fe | Ni | S | 0       | 0       |
|     |       |          | 9     | 4  | 1  | 4 |         |         |
| 4   | D     | 1        | Total | Fe | Ni | S | 0       | 0       |
|     |       |          | 9     | 4  | 1  | 4 |         |         |

- Molecule 5 is XENON (CCD ID: XE) (formula: Xe).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 6        | Total | Xe | 0       | 1       |
|     |       |          | 7     | 7  |         |         |
| 5   | B     | 6        | Total | Xe | 0       | 1       |
|     |       |          | 7     | 7  |         |         |
| 5   | C     | 6        | Total | Xe | 0       | 1       |
|     |       |          | 7     | 7  |         |         |
| 5   | D     | 6        | Total | Xe | 0       | 1       |
|     |       |          | 7     | 7  |         |         |
| 5   | M     | 3        | Total | Xe | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 5   | N     | 4        | Total | Xe | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 5   | O     | 3        | Total | Xe | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 5   | P     | 4        | Total | Xe | 0       | 0       |
|     |       |          | 4     | 4  |         |         |

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 6   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 6   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 6   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 6   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 6   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 6   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 6   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 6   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 6   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 6   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 6   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

- Molecule 7 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 7   | M     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 7   | N     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 7   | O     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 7   | P     | 1        | Total Cu<br>1 1 | 0       | 0       |

- Molecule 8 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 8   | M     | 1        | Total Ni<br>1 1 | 0       | 0       |
| 8   | N     | 1        | Total Ni<br>1 1 | 0       | 0       |
| 8   | O     | 1        | Total Ni<br>1 1 | 0       | 0       |
| 8   | P     | 1        | Total Ni<br>1 1 | 0       | 0       |

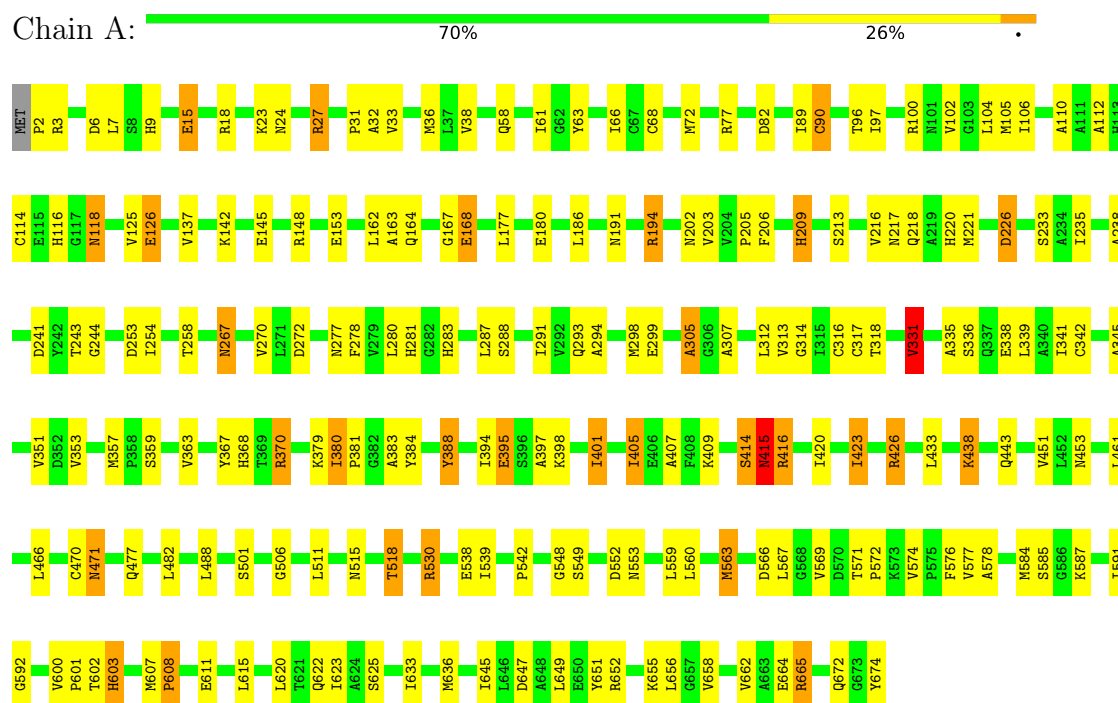
- Molecule 9 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 9   | A     | 168      | Total O<br>168 168 | 0       | 0       |
| 9   | B     | 220      | Total O<br>220 220 | 0       | 0       |
| 9   | C     | 130      | Total O<br>130 130 | 0       | 0       |
| 9   | D     | 105      | Total O<br>105 105 | 0       | 0       |
| 9   | M     | 201      | Total O<br>201 201 | 0       | 0       |
| 9   | N     | 222      | Total O<br>222 222 | 0       | 0       |
| 9   | O     | 27       | Total O<br>27 27   | 0       | 0       |
| 9   | P     | 80       | Total O<br>80 80   | 0       | 0       |

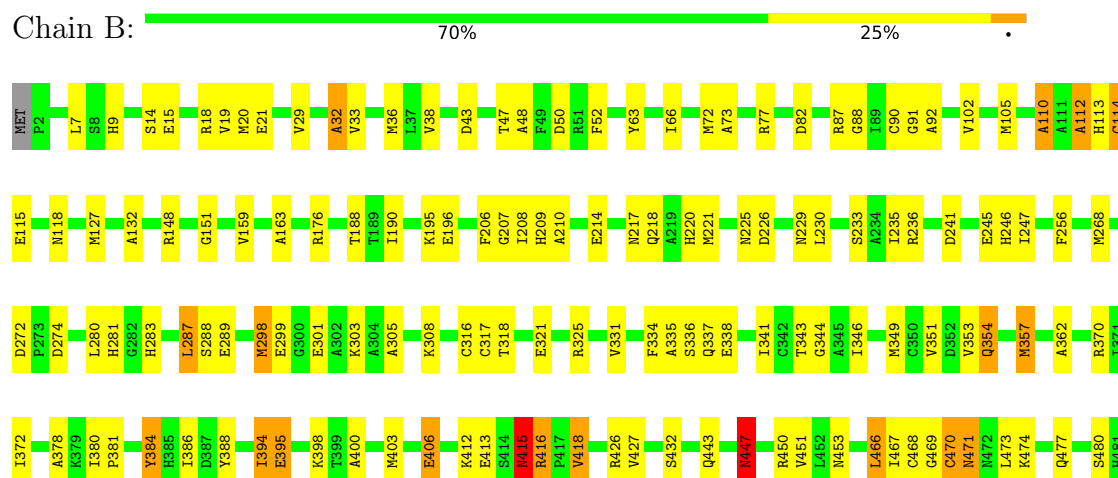
### 3 Residue-property plots

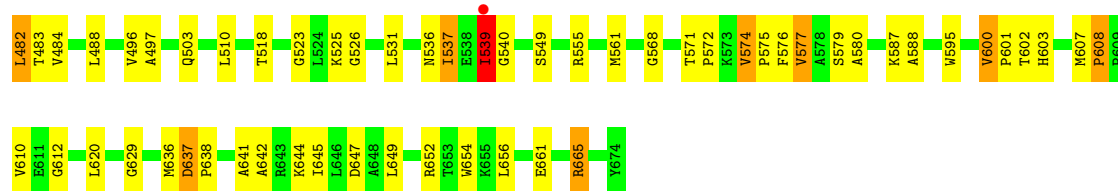
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit beta



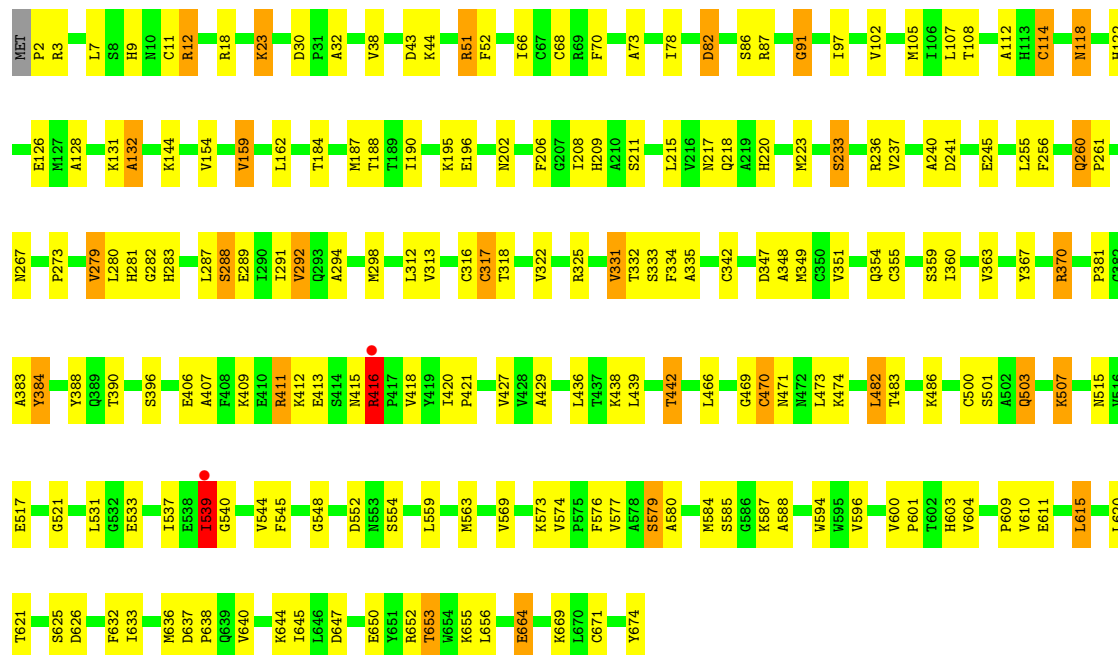
- Molecule 1: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit beta





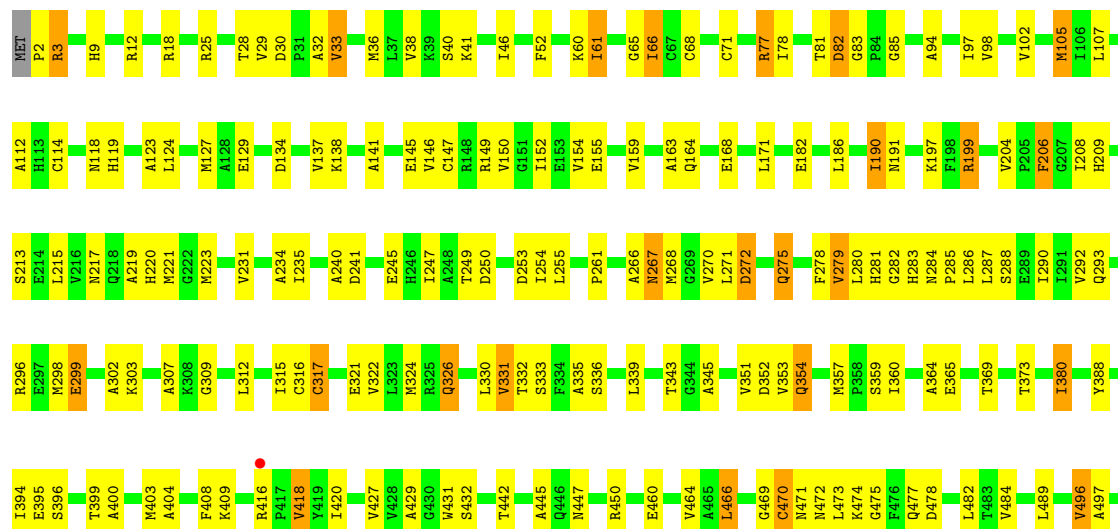
• Molecule 1: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit beta

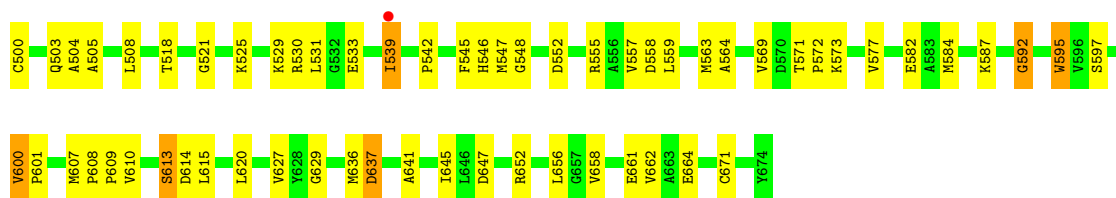
Chain C: 70% 25% .



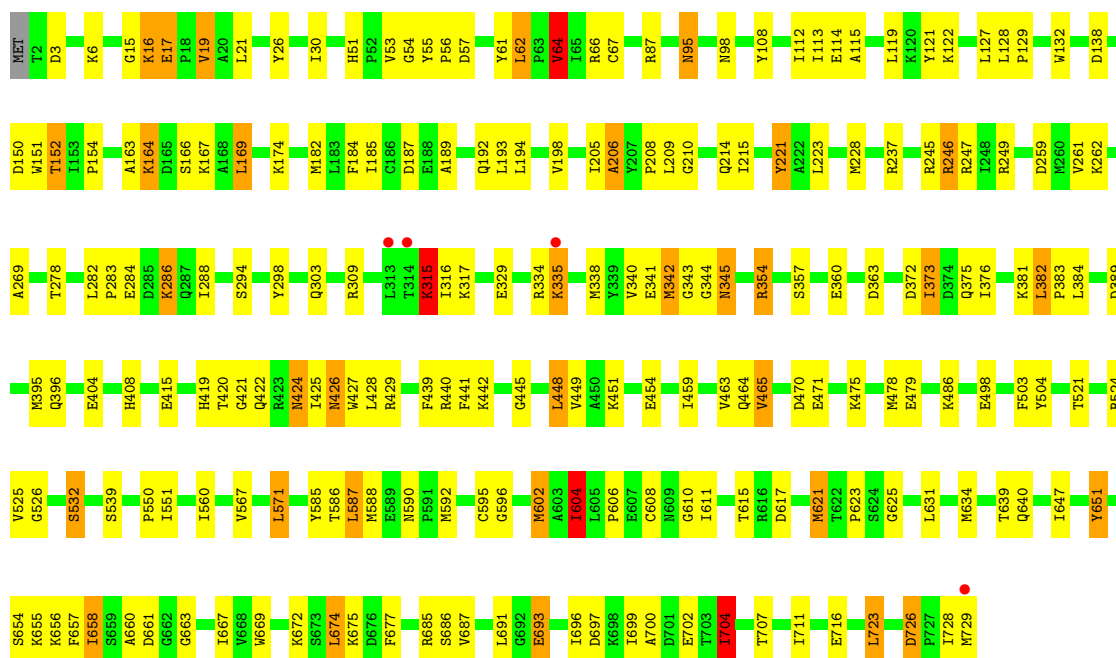
• Molecule 1: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit beta

Chain D: 64% 32% .

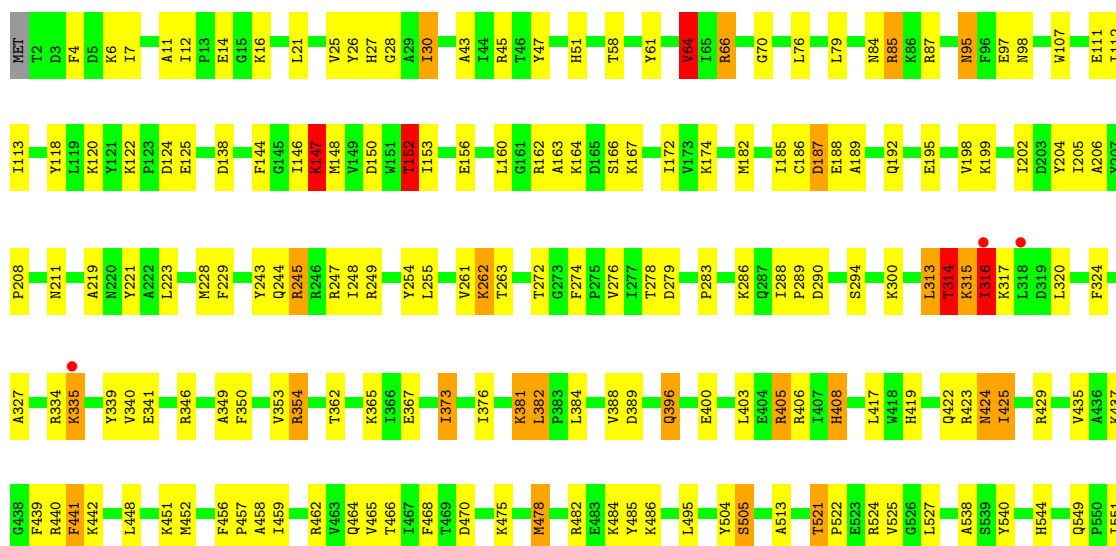


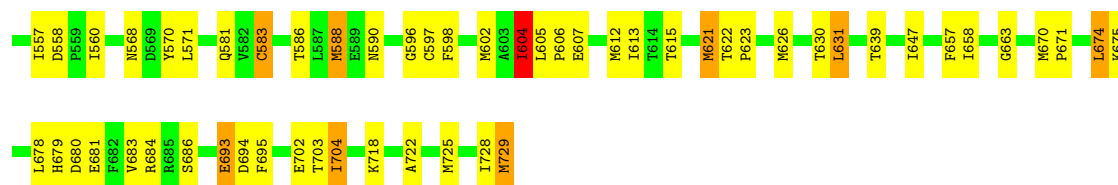


• Molecule 2: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit alpha

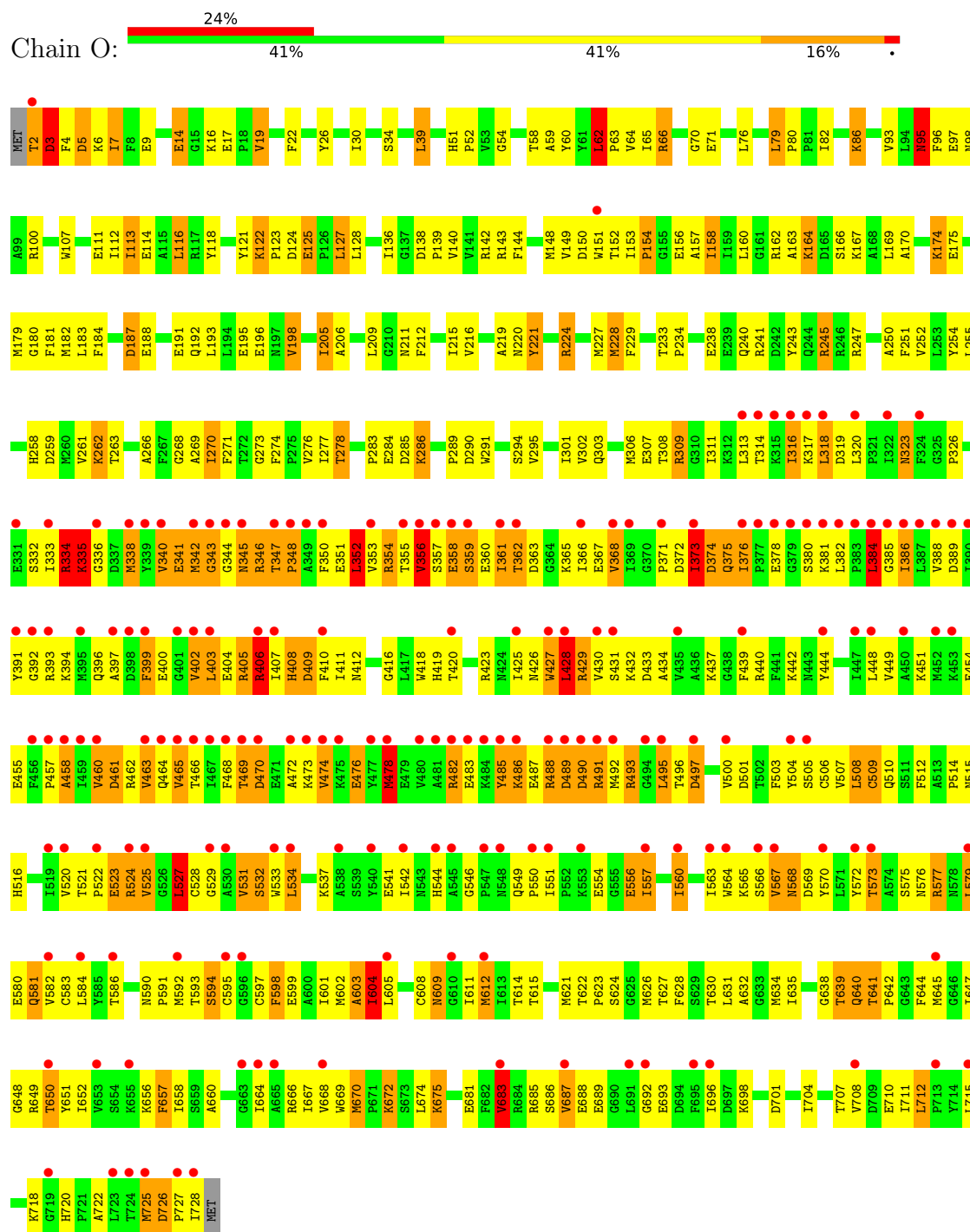


• Molecule 2: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit alpha

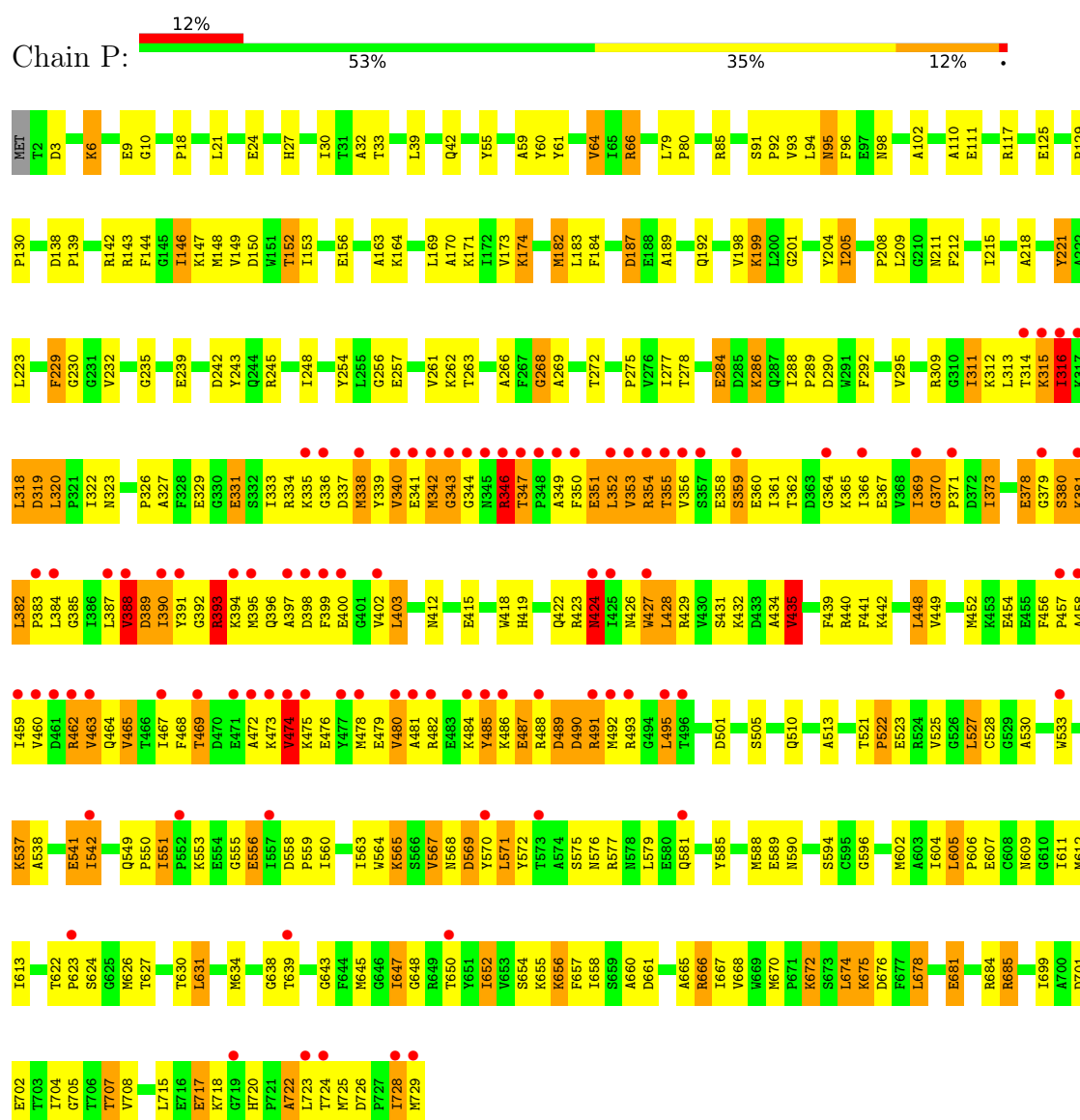




• Molecule 2: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit alpha



• Molecule 2: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit alpha



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 99.54Å 136.60Å 141.75Å<br>101.29° 109.22° 103.91°           | Depositor        |
| Resolution (Å)                                                          | 49.00 – 2.51<br>49.00 – 2.51                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.1 (49.00-2.51)<br>96.1 (49.00-2.51)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.08                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.67 (at 2.48Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.178 , 0.250<br>0.179 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 29.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.322                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 41.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 44706                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 31.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, SF4, XE, GOL, CU1, XCC

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     | 1.58         | 29/5187 (0.6%)   | 1.44        | 30/7028 (0.4%)   |
| 1   | B     | 1.60         | 34/5187 (0.7%)   | 1.43        | 35/7028 (0.5%)   |
| 1   | C     | 1.54         | 19/5187 (0.4%)   | 1.44        | 32/7028 (0.5%)   |
| 1   | D     | 1.47         | 15/5187 (0.3%)   | 1.44        | 49/7028 (0.7%)   |
| 2   | M     | 1.49         | 24/5874 (0.4%)   | 1.36        | 39/7954 (0.5%)   |
| 2   | N     | 1.51         | 27/5874 (0.5%)   | 1.41        | 48/7954 (0.6%)   |
| 2   | O     | 1.40         | 15/5859 (0.3%)   | 1.36        | 42/7937 (0.5%)   |
| 2   | P     | 1.39         | 16/5874 (0.3%)   | 1.36        | 43/7954 (0.5%)   |
| All | All   | 1.50         | 179/44229 (0.4%) | 1.41        | 318/59911 (0.5%) |

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   | A     | 0                   | 1                   |
| 1   | B     | 0                   | 1                   |
| 1   | C     | 0                   | 2                   |
| 1   | D     | 0                   | 1                   |
| 2   | N     | 0                   | 1                   |
| 2   | P     | 0                   | 2                   |
| All | All   | 0                   | 8                   |

All (179) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 383 | ALA  | CA-CB | -9.21 | 1.37        | 1.53     |
| 1   | A     | 397 | ALA  | CA-CB | -9.02 | 1.39        | 1.53     |
| 1   | C     | 363 | VAL  | CA-CB | -8.55 | 1.45        | 1.54     |
| 2   | P     | 208 | PRO  | C-O   | 8.10  | 1.30        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 3   | ARG  | CA-C  | 7.96  | 1.62        | 1.52     |
| 1   | D     | 484 | VAL  | CA-CB | 7.93  | 1.62        | 1.54     |
| 2   | M     | 504 | TYR  | CA-C  | -7.86 | 1.43        | 1.52     |
| 1   | A     | 168 | GLU  | CG-CD | 7.48  | 1.70        | 1.52     |
| 1   | B     | 113 | HIS  | CA-C  | -7.47 | 1.42        | 1.52     |
| 2   | O     | 683 | VAL  | CA-CB | 7.37  | 1.62        | 1.54     |
| 2   | M     | 269 | ALA  | CA-CB | 7.35  | 1.64        | 1.53     |
| 2   | N     | 538 | ALA  | CA-CB | -7.16 | 1.42        | 1.53     |
| 2   | N     | 324 | PHE  | CA-C  | -7.15 | 1.44        | 1.52     |
| 2   | N     | 521 | THR  | CA-CB | 7.09  | 1.62        | 1.54     |
| 2   | O     | 113 | ILE  | CA-CB | -6.98 | 1.46        | 1.54     |
| 1   | C     | 132 | ALA  | CA-CB | -6.90 | 1.45        | 1.53     |
| 1   | A     | 591 | ILE  | CA-CB | -6.87 | 1.45        | 1.54     |
| 1   | B     | 305 | ALA  | CA-CB | -6.85 | 1.42        | 1.53     |
| 1   | A     | 578 | ALA  | CA-CB | -6.84 | 1.41        | 1.53     |
| 1   | B     | 92  | ALA  | CA-CB | -6.79 | 1.42        | 1.53     |
| 1   | D     | 231 | VAL  | CA-CB | -6.77 | 1.46        | 1.54     |
| 2   | N     | 97  | GLU  | N-CA  | -6.75 | 1.38        | 1.46     |
| 2   | M     | 61  | TYR  | C-O   | -6.73 | 1.17        | 1.24     |
| 2   | P     | 129 | PRO  | CA-C  | -6.69 | 1.46        | 1.52     |
| 2   | M     | 329 | GLU  | C-O   | -6.63 | 1.16        | 1.24     |
| 1   | C     | 288 | SER  | N-CA  | -6.62 | 1.37        | 1.46     |
| 2   | N     | 320 | LEU  | N-CA  | -6.58 | 1.41        | 1.46     |
| 2   | N     | 294 | SER  | N-CA  | -6.57 | 1.38        | 1.46     |
| 1   | B     | 214 | GLU  | CA-C  | 6.56  | 1.61        | 1.52     |
| 2   | M     | 590 | ASN  | C-O   | -6.56 | 1.20        | 1.23     |
| 1   | A     | 542 | PRO  | C-O   | -6.52 | 1.17        | 1.24     |
| 2   | N     | 279 | ASP  | C-O   | -6.49 | 1.15        | 1.24     |
| 2   | P     | 232 | VAL  | CA-CB | -6.49 | 1.47        | 1.54     |
| 1   | B     | 539 | ILE  | CA-CB | 6.42  | 1.63        | 1.54     |
| 2   | O     | 520 | VAL  | CA-CB | 6.42  | 1.61        | 1.53     |
| 1   | A     | 407 | ALA  | CA-CB | -6.38 | 1.42        | 1.53     |
| 1   | D     | 33  | VAL  | CA-CB | 6.35  | 1.63        | 1.54     |
| 1   | D     | 78  | ILE  | CA-C  | -6.34 | 1.45        | 1.52     |
| 1   | B     | 378 | ALA  | CA-CB | 6.32  | 1.61        | 1.52     |
| 1   | C     | 548 | GLY  | C-O   | -6.31 | 1.19        | 1.24     |
| 1   | D     | 641 | ALA  | CA-CB | -6.30 | 1.43        | 1.53     |
| 2   | O     | 542 | ILE  | CA-CB | 6.29  | 1.61        | 1.54     |
| 1   | A     | 379 | LYS  | C-O   | 6.25  | 1.31        | 1.23     |
| 2   | P     | 622 | THR  | CA-CB | 6.25  | 1.63        | 1.54     |
| 2   | O     | 687 | VAL  | CA-CB | 6.21  | 1.62        | 1.54     |
| 1   | A     | 401 | ILE  | CA-CB | -6.18 | 1.47        | 1.54     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 267 | ASN  | CA-C  | -6.17 | 1.44        | 1.52     |
| 1   | C     | 388 | TYR  | C-O   | -6.14 | 1.16        | 1.24     |
| 1   | C     | 580 | ALA  | CA-CB | -6.13 | 1.45        | 1.53     |
| 2   | N     | 316 | ILE  | CA-CB | 6.13  | 1.62        | 1.54     |
| 1   | A     | 164 | GLN  | C-O   | -6.12 | 1.17        | 1.24     |
| 1   | A     | 258 | THR  | CA-C  | -6.12 | 1.45        | 1.52     |
| 2   | P     | 93  | VAL  | CA-C  | -6.12 | 1.45        | 1.52     |
| 2   | P     | 263 | THR  | CA-CB | -6.06 | 1.43        | 1.53     |
| 1   | B     | 349 | MET  | N-CA  | -6.06 | 1.38        | 1.46     |
| 2   | N     | 276 | VAL  | CA-CB | 6.01  | 1.61        | 1.54     |
| 2   | M     | 206 | ALA  | CA-CB | -5.98 | 1.43        | 1.53     |
| 2   | M     | 246 | ARG  | C-O   | -5.97 | 1.17        | 1.24     |
| 2   | N     | 186 | CYS  | N-CA  | -5.96 | 1.38        | 1.46     |
| 2   | N     | 465 | VAL  | CA-CB | 5.96  | 1.62        | 1.54     |
| 2   | M     | 138 | ASP  | CA-C  | 5.95  | 1.60        | 1.52     |
| 2   | N     | 113 | ILE  | CA-CB | -5.94 | 1.47        | 1.54     |
| 1   | B     | 447 | ASN  | C-O   | 5.94  | 1.30        | 1.24     |
| 2   | N     | 25  | VAL  | CA-CB | -5.93 | 1.47        | 1.54     |
| 2   | O     | 311 | ILE  | CA-CB | 5.92  | 1.59        | 1.53     |
| 2   | N     | 604 | ILE  | CA-CB | 5.91  | 1.60        | 1.54     |
| 1   | A     | 305 | ALA  | CA-CB | -5.89 | 1.43        | 1.53     |
| 1   | A     | 63  | TYR  | C-O   | -5.88 | 1.17        | 1.24     |
| 2   | M     | 53  | VAL  | CA-CB | 5.83  | 1.63        | 1.54     |
| 1   | B     | 196 | GLU  | CG-CD | 5.82  | 1.66        | 1.52     |
| 2   | P     | 94  | LEU  | C-O   | -5.78 | 1.17        | 1.24     |
| 2   | N     | 683 | VAL  | CA-CB | 5.78  | 1.61        | 1.54     |
| 1   | D     | 546 | HIS  | N-CA  | -5.77 | 1.39        | 1.46     |
| 2   | P     | 311 | ILE  | CA-CB | 5.76  | 1.61        | 1.54     |
| 1   | B     | 21  | GLU  | N-CA  | 5.76  | 1.50        | 1.46     |
| 1   | B     | 188 | THR  | CA-CB | 5.75  | 1.63        | 1.53     |
| 1   | D     | 254 | ILE  | CA-CB | -5.75 | 1.47        | 1.54     |
| 2   | P     | 316 | ILE  | CA-CB | 5.74  | 1.62        | 1.54     |
| 1   | A     | 353 | VAL  | C-O   | -5.74 | 1.18        | 1.24     |
| 1   | B     | 539 | ILE  | CA-C  | 5.73  | 1.60        | 1.52     |
| 2   | N     | 525 | VAL  | CA-CB | 5.70  | 1.59        | 1.54     |
| 1   | B     | 568 | GLY  | CA-C  | 5.69  | 1.57        | 1.51     |
| 1   | B     | 225 | ASN  | N-CA  | -5.68 | 1.40        | 1.46     |
| 2   | O     | 356 | VAL  | CA-CB | 5.66  | 1.62        | 1.54     |
| 2   | M     | 465 | VAL  | CA-CB | 5.66  | 1.61        | 1.54     |
| 1   | B     | 38  | VAL  | CA-CB | 5.64  | 1.61        | 1.54     |
| 1   | B     | 32  | ALA  | CA-CB | -5.64 | 1.44        | 1.53     |
| 2   | O     | 508 | LEU  | C-O   | 5.63  | 1.28        | 1.23     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | M     | 404 | GLU  | CA-C   | -5.62 | 1.45        | 1.52     |
| 2   | P     | 218 | ALA  | CA-CB  | -5.60 | 1.44        | 1.53     |
| 1   | B     | 21  | GLU  | C-O    | -5.60 | 1.21        | 1.23     |
| 2   | P     | 173 | VAL  | CA-CB  | -5.59 | 1.47        | 1.54     |
| 1   | A     | 3   | ARG  | C-O    | -5.58 | 1.17        | 1.24     |
| 2   | N     | 120 | LYS  | CE-NZ  | 5.58  | 1.66        | 1.49     |
| 1   | A     | 90  | CYS  | N-CA   | 5.57  | 1.53        | 1.46     |
| 2   | N     | 172 | ILE  | CA-CB  | -5.56 | 1.47        | 1.54     |
| 1   | C     | 610 | VAL  | CA-CB  | -5.55 | 1.48        | 1.54     |
| 2   | M     | 288 | ILE  | N-CA   | -5.55 | 1.39        | 1.46     |
| 2   | M     | 524 | ARG  | C-O    | 5.54  | 1.30        | 1.24     |
| 1   | C     | 128 | ALA  | C-O    | -5.51 | 1.17        | 1.24     |
| 1   | A     | 61  | ILE  | C-O    | -5.50 | 1.18        | 1.24     |
| 1   | B     | 210 | ALA  | CA-C   | 5.50  | 1.60        | 1.52     |
| 1   | C     | 279 | VAL  | CA-CB  | -5.48 | 1.47        | 1.54     |
| 1   | B     | 577 | VAL  | CA-CB  | 5.48  | 1.64        | 1.55     |
| 1   | A     | 314 | GLY  | N-CA   | 5.47  | 1.50        | 1.44     |
| 1   | B     | 362 | ALA  | CA-CB  | -5.46 | 1.44        | 1.53     |
| 1   | A     | 243 | THR  | CA-CB  | -5.46 | 1.44        | 1.53     |
| 2   | O     | 355 | THR  | CA-C   | 5.46  | 1.59        | 1.53     |
| 1   | B     | 229 | ASN  | C-O    | -5.45 | 1.17        | 1.24     |
| 1   | D     | 163 | ALA  | N-CA   | -5.45 | 1.39        | 1.46     |
| 1   | A     | 383 | ALA  | CA-CB  | -5.44 | 1.41        | 1.53     |
| 2   | O     | 557 | ILE  | CA-CB  | 5.44  | 1.61        | 1.54     |
| 2   | N     | 202 | ILE  | C-O    | -5.43 | 1.18        | 1.24     |
| 2   | P     | 724 | THR  | CA-CB  | 5.42  | 1.62        | 1.53     |
| 2   | O     | 507 | VAL  | C-O    | 5.39  | 1.30        | 1.24     |
| 1   | B     | 482 | LEU  | C-O    | -5.39 | 1.17        | 1.24     |
| 1   | B     | 523 | GLY  | C-O    | 5.38  | 1.30        | 1.23     |
| 2   | M     | 315 | LYS  | N-CA   | 5.36  | 1.53        | 1.46     |
| 1   | D     | 119 | HIS  | CA-C   | 5.34  | 1.59        | 1.52     |
| 1   | A     | 163 | ALA  | N-CA   | -5.33 | 1.39        | 1.46     |
| 2   | M     | 19  | VAL  | C-O    | -5.33 | 1.18        | 1.24     |
| 1   | B     | 272 | ASP  | CA-C   | 5.32  | 1.57        | 1.52     |
| 1   | B     | 287 | LEU  | CG-CD1 | 5.30  | 1.70        | 1.52     |
| 1   | B     | 418 | VAL  | C-O    | -5.30 | 1.18        | 1.24     |
| 1   | B     | 112 | ALA  | CA-CB  | 5.28  | 1.61        | 1.53     |
| 1   | C     | 255 | LEU  | N-CA   | 5.28  | 1.53        | 1.46     |
| 1   | D     | 571 | THR  | CA-C   | 5.28  | 1.59        | 1.52     |
| 2   | P     | 32  | ALA  | CA-C   | 5.26  | 1.59        | 1.52     |
| 2   | M     | 303 | GLN  | N-CA   | -5.23 | 1.40        | 1.46     |
| 1   | B     | 384 | TYR  | CA-C   | -5.23 | 1.46        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 347 | ASP  | CA-CB  | -5.23 | 1.44        | 1.53     |
| 2   | O     | 270 | ILE  | CA-CB  | -5.22 | 1.48        | 1.54     |
| 1   | A     | 82  | ASP  | CB-CG  | -5.21 | 1.39        | 1.52     |
| 1   | A     | 77  | ARG  | C-O    | -5.20 | 1.17        | 1.23     |
| 2   | M     | 286 | LYS  | CA-C   | 5.20  | 1.59        | 1.52     |
| 1   | C     | 473 | LEU  | CA-C   | 5.20  | 1.59        | 1.52     |
| 2   | N     | 504 | TYR  | CA-C   | -5.20 | 1.46        | 1.52     |
| 1   | A     | 226 | ASP  | C-O    | -5.19 | 1.18        | 1.24     |
| 1   | A     | 202 | ASN  | CA-C   | -5.19 | 1.46        | 1.53     |
| 2   | O     | 650 | THR  | CA-CB  | 5.18  | 1.62        | 1.53     |
| 2   | N     | 30  | ILE  | CA-CB  | -5.17 | 1.48        | 1.54     |
| 2   | O     | 39  | LEU  | CA-C   | -5.17 | 1.46        | 1.52     |
| 2   | N     | 583 | CYS  | N-CA   | -5.17 | 1.39        | 1.46     |
| 2   | N     | 524 | ARG  | CZ-NH2 | 5.16  | 1.40        | 1.33     |
| 2   | N     | 702 | GLU  | CB-CG  | -5.15 | 1.36        | 1.52     |
| 1   | B     | 574 | VAL  | C-O    | -5.15 | 1.18        | 1.24     |
| 2   | M     | 210 | GLY  | C-O    | 5.15  | 1.27        | 1.24     |
| 2   | N     | 28  | GLY  | C-O    | -5.13 | 1.17        | 1.23     |
| 1   | C     | 32  | ALA  | CA-CB  | -5.12 | 1.45        | 1.53     |
| 1   | D     | 77  | ARG  | CA-C   | -5.12 | 1.46        | 1.52     |
| 1   | D     | 247 | ILE  | C-O    | -5.11 | 1.18        | 1.24     |
| 1   | A     | 548 | GLY  | N-CA   | 5.11  | 1.50        | 1.45     |
| 2   | M     | 595 | CYS  | C-O    | -5.11 | 1.19        | 1.23     |
| 1   | B     | 247 | ILE  | CB-CG2 | 5.11  | 1.69        | 1.52     |
| 1   | C     | 184 | THR  | CA-CB  | -5.10 | 1.45        | 1.53     |
| 2   | M     | 54  | GLY  | N-CA   | 5.09  | 1.49        | 1.45     |
| 2   | N     | 263 | THR  | N-CA   | -5.09 | 1.40        | 1.46     |
| 1   | A     | 116 | HIS  | C-O    | -5.08 | 1.17        | 1.24     |
| 2   | P     | 292 | PHE  | CA-C   | -5.08 | 1.47        | 1.53     |
| 2   | M     | 550 | PRO  | CA-C   | -5.07 | 1.47        | 1.52     |
| 1   | C     | 292 | VAL  | CA-CB  | -5.07 | 1.48        | 1.54     |
| 1   | B     | 406 | GLU  | CA-C   | -5.07 | 1.46        | 1.52     |
| 1   | D     | 627 | VAL  | N-CA   | -5.07 | 1.40        | 1.46     |
| 1   | A     | 209 | HIS  | C-O    | 5.06  | 1.30        | 1.24     |
| 2   | P     | 32  | ALA  | CA-CB  | -5.05 | 1.45        | 1.53     |
| 2   | M     | 113 | ILE  | C-O    | -5.05 | 1.18        | 1.24     |
| 2   | M     | 639 | THR  | CA-C   | 5.04  | 1.59        | 1.52     |
| 1   | D     | 464 | VAL  | C-O    | -5.04 | 1.19        | 1.24     |
| 2   | N     | 11  | ALA  | CA-CB  | -5.04 | 1.45        | 1.53     |
| 1   | B     | 415 | ASN  | CA-C   | 5.04  | 1.60        | 1.53     |
| 1   | B     | 610 | VAL  | CB-CG2 | 5.04  | 1.69        | 1.52     |
| 1   | B     | 246 | HIS  | N-CA   | -5.04 | 1.39        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 203 | VAL  | C-N   | 5.03  | 1.39        | 1.33     |
| 1   | C     | 580 | ALA  | CA-C  | -5.03 | 1.47        | 1.52     |
| 1   | C     | 237 | VAL  | CA-CB | -5.03 | 1.48        | 1.54     |
| 1   | A     | 216 | VAL  | N-CA  | -5.02 | 1.40        | 1.46     |
| 2   | P     | 55  | TYR  | CA-C  | -5.02 | 1.46        | 1.52     |
| 2   | O     | 532 | SER  | C-O   | 5.01  | 1.30        | 1.23     |
| 2   | M     | 288 | ILE  | CA-CB | -5.01 | 1.47        | 1.54     |

All (318) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|--------|------|---------|--------|-------------|----------|
| 1   | C     | 416    | ARG  | CA-C-N  | -16.11 | 104.52      | 120.31   |
| 1   | C     | 416    | ARG  | C-N-CA  | -16.11 | 104.52      | 120.31   |
| 1   | D     | 38     | VAL  | N-CA-C  | -11.73 | 99.44       | 110.82   |
| 1   | A     | 331    | VAL  | CB-CA-C | -10.49 | 98.18       | 111.92   |
| 2   | O     | 347    | THR  | CA-C-N  | 10.18  | 132.57      | 119.84   |
| 2   | O     | 347    | THR  | C-N-CA  | 10.18  | 132.57      | 119.84   |
| 1   | C     | 331    | VAL  | CB-CA-C | -10.03 | 98.90       | 112.04   |
| 2   | O     | 546    | GLY  | CA-C-N  | 9.53   | 130.70      | 120.12   |
| 2   | O     | 546    | GLY  | C-N-CA  | 9.53   | 130.70      | 120.12   |
| 1   | C     | 539[A] | ILE  | N-CA-C  | 9.47   | 120.29      | 110.72   |
| 2   | P     | 675    | LYS  | N-CA-C  | -9.38  | 100.61      | 111.03   |
| 1   | D     | 272    | ASP  | CA-C-N  | -8.94  | 110.58      | 119.87   |
| 1   | D     | 272    | ASP  | C-N-CA  | -8.94  | 110.58      | 119.87   |
| 1   | D     | 365    | GLU  | N-CA-C  | -8.90  | 102.20      | 113.23   |
| 2   | O     | 343    | GLY  | N-CA-C  | 8.83   | 122.36      | 110.43   |
| 1   | A     | 395    | GLU  | N-CA-C  | 8.78   | 120.85      | 111.28   |
| 1   | A     | 471    | ASN  | N-CA-C  | -8.70  | 96.66       | 110.14   |
| 2   | P     | 102    | ALA  | N-CA-C  | -8.69  | 102.11      | 112.89   |
| 1   | C     | 521    | GLY  | N-CA-C  | -8.46  | 100.91      | 112.25   |
| 2   | P     | 30     | ILE  | N-CA-C  | -8.45  | 102.31      | 110.42   |
| 2   | N     | 456    | PHE  | CA-C-N  | -8.39  | 111.38      | 119.85   |
| 2   | N     | 456    | PHE  | C-N-CA  | -8.39  | 111.38      | 119.85   |
| 1   | A     | 380    | ILE  | CA-C-N  | -8.33  | 111.39      | 119.89   |
| 1   | A     | 380    | ILE  | C-N-CA  | -8.33  | 111.39      | 119.89   |
| 2   | O     | 79     | LEU  | CA-C-N  | -8.28  | 111.85      | 120.38   |
| 2   | O     | 79     | LEU  | C-N-CA  | -8.28  | 111.85      | 120.38   |
| 1   | D     | 284    | ASN  | CA-C-N  | -7.84  | 111.75      | 120.45   |
| 1   | D     | 284    | ASN  | C-N-CA  | -7.84  | 111.75      | 120.45   |
| 1   | D     | 475    | GLY  | N-CA-C  | -7.83  | 99.12       | 111.18   |
| 1   | C     | 349    | MET  | N-CA-C  | -7.82  | 96.15       | 108.90   |
| 2   | O     | 309    | ARG  | N-CA-C  | -7.81  | 102.72      | 111.07   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | C     | 615 | LEU  | N-CA-C   | -7.71 | 102.82      | 111.14   |
| 1   | D     | 141 | ALA  | N-CA-C   | -7.64 | 103.03      | 111.36   |
| 2   | O     | 59  | ALA  | N-CA-C   | -7.58 | 101.91      | 113.89   |
| 2   | N     | 703 | THR  | CA-C-N   | -7.55 | 115.33      | 122.66   |
| 2   | N     | 703 | THR  | C-N-CA   | -7.55 | 115.33      | 122.66   |
| 2   | N     | 376 | ILE  | CA-C-N   | -7.53 | 112.93      | 120.31   |
| 2   | N     | 376 | ILE  | C-N-CA   | -7.53 | 112.93      | 120.31   |
| 2   | N     | 621 | MET  | CG-SD-CE | -7.53 | 84.33       | 100.90   |
| 2   | M     | 376 | ILE  | CA-C-N   | -7.52 | 111.64      | 120.13   |
| 2   | M     | 376 | ILE  | C-N-CA   | -7.52 | 111.64      | 120.13   |
| 2   | N     | 382 | LEU  | CA-C-N   | -7.50 | 112.97      | 120.31   |
| 2   | N     | 382 | LEU  | C-N-CA   | -7.50 | 112.97      | 120.31   |
| 1   | B     | 230 | LEU  | N-CA-C   | 7.37  | 119.31      | 111.28   |
| 2   | M     | 697 | ASP  | N-CA-C   | -7.36 | 104.45      | 113.50   |
| 1   | C     | 664 | GLU  | N-CA-C   | -7.34 | 102.45      | 111.40   |
| 1   | C     | 51  | ARG  | N-CA-C   | -7.26 | 103.40      | 111.82   |
| 1   | D     | 331 | VAL  | CB-CA-C  | -7.24 | 102.54      | 112.02   |
| 1   | D     | 331 | VAL  | N-CA-C   | 7.23  | 117.33      | 110.53   |
| 1   | B     | 537 | ILE  | CB-CA-C  | 7.22  | 119.45      | 111.80   |
| 2   | N     | 702 | GLU  | CB-CA-C  | -7.21 | 96.47       | 110.46   |
| 2   | N     | 147 | LYS  | N-CA-C   | -7.18 | 104.78      | 113.97   |
| 2   | N     | 631 | LEU  | N-CA-C   | -7.16 | 103.55      | 111.36   |
| 2   | O     | 573 | THR  | N-CA-C   | 7.16  | 119.16      | 111.36   |
| 1   | D     | 629 | GLY  | N-CA-C   | -7.11 | 106.62      | 115.08   |
| 2   | M     | 687 | VAL  | N-CA-C   | -7.08 | 103.43      | 110.30   |
| 2   | O     | 352 | LEU  | N-CA-C   | 7.04  | 119.56      | 108.79   |
| 1   | B     | 163 | ALA  | N-CA-C   | -7.03 | 103.61      | 111.28   |
| 2   | N     | 704 | ILE  | CB-CA-C  | 7.03  | 118.05      | 111.30   |
| 1   | B     | 344 | GLY  | N-CA-C   | -7.02 | 106.09      | 115.21   |
| 1   | D     | 548 | GLY  | N-CA-C   | 7.00  | 118.63      | 111.56   |
| 2   | M     | 728 | ILE  | N-CA-C   | -6.97 | 102.10      | 111.44   |
| 1   | C     | 38  | VAL  | N-CA-C   | -6.96 | 103.99      | 110.53   |
| 1   | D     | 394 | ILE  | N-CA-C   | 6.88  | 117.03      | 110.42   |
| 2   | N     | 670 | MET  | CA-C-N   | -6.87 | 112.91      | 119.85   |
| 2   | N     | 670 | MET  | C-N-CA   | -6.87 | 112.91      | 119.85   |
| 1   | D     | 81  | THR  | N-CA-C   | -6.86 | 105.06      | 113.50   |
| 1   | B     | 66  | ILE  | N-CA-C   | 6.85  | 118.73      | 112.29   |
| 1   | B     | 29  | VAL  | N-CA-C   | -6.83 | 105.68      | 112.17   |
| 1   | C     | 70  | PHE  | N-CA-C   | 6.82  | 121.19      | 113.01   |
| 1   | A     | 38  | VAL  | N-CA-C   | -6.82 | 104.12      | 110.53   |
| 2   | P     | 153 | ILE  | N-CA-C   | -6.81 | 100.81      | 107.55   |
| 1   | D     | 442 | THR  | N-CA-C   | -6.74 | 104.32      | 112.54   |

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| Mol | Chain | Res    | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1   | A     | 563    | MET  | CG-SD-CE  | -6.74 | 86.08       | 100.90   |
| 2   | O     | 384    | LEU  | N-CA-C    | 6.69  | 120.37      | 109.59   |
| 2   | P     | 59     | ALA  | N-CA-C    | -6.68 | 103.52      | 112.94   |
| 1   | A     | 291    | ILE  | N-CA-C    | -6.65 | 103.84      | 110.62   |
| 1   | B     | 642    | ALA  | N-CA-C    | -6.60 | 104.16      | 111.82   |
| 2   | N     | 459    | ILE  | N-CA-C    | -6.60 | 102.84      | 111.09   |
| 1   | B     | 115    | GLU  | N-CA-C    | -6.58 | 104.10      | 111.28   |
| 1   | C     | 240    | ALA  | N-CA-C    | -6.55 | 104.22      | 111.36   |
| 1   | B     | 110    | ALA  | N-CA-C    | -6.55 | 104.06      | 111.07   |
| 2   | P     | 91     | SER  | CA-C-N    | -6.53 | 114.17      | 120.83   |
| 2   | P     | 91     | SER  | C-N-CA    | -6.53 | 114.17      | 120.83   |
| 2   | P     | 268    | GLY  | N-CA-C    | -6.51 | 104.64      | 113.37   |
| 1   | A     | 623    | ILE  | N-CA-C    | 6.51  | 117.26      | 110.62   |
| 2   | M     | 459    | ILE  | N-CA-C    | -6.49 | 102.74      | 111.44   |
| 1   | C     | 355    | CYS  | CA-C-N    | -6.46 | 114.63      | 122.90   |
| 1   | C     | 355    | CYS  | C-N-CA    | -6.46 | 114.63      | 122.90   |
| 1   | B     | 236    | ARG  | NE-CZ-NH2 | -6.46 | 113.39      | 119.20   |
| 1   | D     | 206    | PHE  | N-CA-C    | -6.46 | 101.68      | 111.56   |
| 1   | D     | 240    | ALA  | N-CA-C    | -6.44 | 104.34      | 111.36   |
| 2   | N     | 70     | GLY  | N-CA-C    | 6.44  | 122.74      | 115.08   |
| 1   | A     | 388    | TYR  | N-CA-C    | 6.43  | 119.55      | 109.96   |
| 1   | C     | 82     | ASP  | N-CA-C    | 6.43  | 117.93      | 108.86   |
| 1   | A     | 438    | LYS  | N-CA-C    | -6.42 | 103.40      | 111.11   |
| 2   | N     | 513    | ALA  | CA-C-N    | 6.40  | 126.08      | 119.56   |
| 2   | N     | 513    | ALA  | C-N-CA    | 6.40  | 126.08      | 119.56   |
| 1   | B     | 357    | MET  | CA-C-N    | -6.38 | 113.23      | 119.87   |
| 1   | B     | 357    | MET  | C-N-CA    | -6.38 | 113.23      | 119.87   |
| 2   | O     | 221    | TYR  | N-CA-C    | -6.38 | 103.95      | 111.03   |
| 2   | O     | 70     | GLY  | CA-C-N    | -6.36 | 112.68      | 122.09   |
| 2   | O     | 70     | GLY  | C-N-CA    | -6.36 | 112.68      | 122.09   |
| 2   | O     | 3      | ASP  | N-CA-C    | -6.34 | 105.37      | 113.23   |
| 1   | A     | 307    | ALA  | N-CA-C    | -6.33 | 101.57      | 110.50   |
| 1   | B     | 665[A] | ARG  | N-CA-C    | -6.32 | 103.92      | 111.69   |
| 2   | O     | 465    | VAL  | N-CA-C    | 6.31  | 117.86      | 108.46   |
| 1   | C     | 406    | GLU  | N-CA-C    | -6.30 | 104.41      | 111.28   |
| 2   | O     | 568    | ASN  | N-CA-C    | 6.29  | 118.14      | 111.28   |
| 1   | D     | 359    | SER  | CA-CB-OG  | -6.27 | 98.56       | 111.10   |
| 2   | P     | 551    | ILE  | CA-C-N    | -6.25 | 113.52      | 120.14   |
| 2   | P     | 551    | ILE  | C-N-CA    | -6.25 | 113.52      | 120.14   |
| 2   | O     | 95     | ASN  | N-CA-C    | 6.24  | 116.31      | 108.45   |
| 2   | O     | 62     | LEU  | CA-C-N    | 6.23  | 125.96      | 119.05   |
| 2   | O     | 62     | LEU  | C-N-CA    | 6.23  | 125.96      | 119.05   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | O     | 278 | THR  | N-CA-C    | 6.22  | 118.87      | 109.23   |
| 2   | N     | 248 | ILE  | CA-C-N    | -6.21 | 112.86      | 122.05   |
| 2   | N     | 248 | ILE  | C-N-CA    | -6.21 | 112.86      | 122.05   |
| 2   | M     | 119 | LEU  | N-CA-C    | -6.17 | 105.01      | 112.54   |
| 1   | D     | 29  | VAL  | N-CA-C    | -6.15 | 106.78      | 112.43   |
| 1   | B     | 540 | GLY  | N-CA-C    | -6.14 | 103.45      | 111.37   |
| 1   | D     | 521 | GLY  | N-CA-C    | -6.14 | 103.11      | 112.51   |
| 1   | B     | 608 | PRO  | N-CA-C    | -6.14 | 103.21      | 110.70   |
| 1   | B     | 43  | ASP  | N-CA-C    | -6.12 | 105.80      | 113.20   |
| 2   | O     | 647 | ILE  | N-CA-C    | 6.11  | 117.50      | 108.45   |
| 1   | A     | 530 | ARG  | NE-CZ-NH1 | -6.04 | 115.46      | 121.50   |
| 1   | B     | 151 | GLY  | N-CA-C    | -6.03 | 106.77      | 115.27   |
| 1   | C     | 604 | VAL  | N-CA-C    | -6.02 | 99.38       | 108.17   |
| 2   | O     | 605 | LEU  | CA-C-N    | 6.00  | 126.11      | 119.87   |
| 2   | O     | 605 | LEU  | C-N-CA    | 6.00  | 126.11      | 119.87   |
| 2   | P     | 284 | GLU  | N-CA-C    | -6.00 | 105.44      | 112.89   |
| 1   | D     | 123 | ALA  | N-CA-C    | 6.00  | 117.82      | 111.28   |
| 1   | D     | 317 | CYS  | N-CA-C    | 5.99  | 117.89      | 111.36   |
| 2   | M     | 526 | GLY  | N-CA-C    | -5.94 | 104.41      | 111.36   |
| 2   | O     | 531 | VAL  | N-CA-C    | 5.93  | 116.72      | 108.89   |
| 1   | D     | 445 | ALA  | N-CA-C    | -5.92 | 106.10      | 113.38   |
| 2   | M     | 587 | LEU  | N-CA-C    | -5.91 | 106.03      | 113.72   |
| 2   | N     | 590 | ASN  | CA-C-N    | -5.91 | 114.18      | 120.03   |
| 2   | N     | 590 | ASN  | C-N-CA    | -5.91 | 114.18      | 120.03   |
| 2   | P     | 388 | VAL  | N-CA-C    | 5.91  | 116.61      | 107.99   |
| 2   | M     | 26  | TYR  | N-CA-C    | -5.88 | 104.95      | 111.36   |
| 2   | P     | 92  | PRO  | N-CA-C    | -5.88 | 108.57      | 114.68   |
| 2   | P     | 33  | THR  | N-CA-C    | -5.87 | 105.22      | 112.90   |
| 1   | C     | 442 | THR  | N-CA-C    | -5.84 | 105.65      | 112.89   |
| 2   | M     | 64  | VAL  | N-CA-CB   | 5.84  | 119.34      | 110.58   |
| 2   | P     | 42  | GLN  | N-CA-C    | -5.84 | 104.87      | 112.23   |
| 1   | A     | 163 | ALA  | N-CA-C    | -5.84 | 105.00      | 111.36   |
| 1   | B     | 48  | ALA  | N-CA-C    | 5.84  | 118.39      | 111.33   |
| 1   | A     | 244 | GLY  | N-CA-C    | -5.82 | 105.32      | 112.77   |
| 1   | D     | 592 | GLY  | N-CA-C    | -5.79 | 105.36      | 112.77   |
| 2   | O     | 273 | GLY  | N-CA-C    | 5.79  | 123.59      | 115.43   |
| 2   | N     | 85  | ARG  | CG-CD-NE  | -5.79 | 99.26       | 112.00   |
| 2   | P     | 521 | THR  | CA-C-N    | 5.77  | 127.05      | 119.84   |
| 2   | P     | 521 | THR  | C-N-CA    | 5.77  | 127.05      | 119.84   |
| 2   | P     | 530 | ALA  | N-CA-C    | 5.75  | 117.63      | 111.36   |
| 1   | B     | 612 | GLY  | CA-C-N    | -5.75 | 114.70      | 122.86   |
| 1   | B     | 612 | GLY  | C-N-CA    | -5.75 | 114.70      | 122.86   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | N     | 557 | ILE  | N-CA-C    | -5.74 | 107.30      | 112.12   |
| 2   | P     | 381 | LYS  | N-CA-C    | -5.74 | 100.82      | 108.34   |
| 2   | N     | 118 | TYR  | N-CA-C    | -5.74 | 106.04      | 113.16   |
| 2   | P     | 229 | PHE  | N-CA-C    | -5.74 | 105.05      | 112.68   |
| 1   | D     | 404 | ALA  | N-CA-C    | -5.74 | 104.64      | 111.69   |
| 1   | A     | 66  | ILE  | N-CA-C    | 5.70  | 117.70      | 111.77   |
| 1   | B     | 225 | ASN  | N-CA-C    | -5.70 | 104.55      | 112.30   |
| 1   | B     | 600 | VAL  | N-CA-CB   | -5.70 | 106.33      | 112.37   |
| 1   | A     | 423 | ILE  | N-CA-C    | 5.69  | 116.05      | 107.75   |
| 2   | O     | 241 | ARG  | NE-CZ-NH1 | -5.68 | 115.82      | 121.50   |
| 1   | D     | 60  | LYS  | N-CA-C    | -5.67 | 105.08      | 112.23   |
| 2   | P     | 235 | GLY  | N-CA-C    | -5.67 | 107.94      | 114.69   |
| 2   | O     | 140 | VAL  | N-CA-C    | -5.67 | 104.36      | 112.35   |
| 1   | D     | 542 | PRO  | CA-C-N    | -5.66 | 113.19      | 119.19   |
| 1   | D     | 542 | PRO  | C-N-CA    | -5.66 | 113.19      | 119.19   |
| 1   | D     | 339 | LEU  | CA-CB-CG  | -5.65 | 96.52       | 116.30   |
| 2   | N     | 152 | THR  | N-CA-CB   | 5.65  | 118.92      | 110.22   |
| 2   | M     | 604 | ILE  | CB-CA-C   | -5.64 | 103.85      | 111.63   |
| 2   | O     | 116 | LEU  | N-CA-C    | 5.63  | 117.09      | 111.07   |
| 2   | O     | 455 | GLU  | N-CA-C    | 5.63  | 120.14      | 113.16   |
| 2   | N     | 12  | ILE  | CA-C-N    | 5.61  | 125.52      | 119.85   |
| 2   | N     | 12  | ILE  | C-N-CA    | 5.61  | 125.52      | 119.85   |
| 2   | N     | 505 | SER  | N-CA-C    | -5.59 | 102.25      | 110.52   |
| 1   | A     | 488 | LEU  | N-CA-C    | -5.58 | 105.27      | 111.36   |
| 2   | N     | 441 | PHE  | N-CA-C    | 5.57  | 118.12      | 111.71   |
| 1   | D     | 489 | LEU  | N-CA-C    | -5.57 | 105.21      | 111.28   |
| 2   | M     | 122 | LYS  | CA-C-N    | 5.57  | 125.67      | 119.32   |
| 2   | M     | 122 | LYS  | C-N-CA    | 5.57  | 125.67      | 119.32   |
| 1   | A     | 104 | LEU  | N-CA-C    | -5.56 | 105.30      | 111.36   |
| 2   | N     | 64  | VAL  | N-CA-CB   | 5.55  | 118.09      | 110.54   |
| 2   | N     | 245 | ARG  | CB-CG-CD  | 5.55  | 124.06      | 111.30   |
| 1   | D     | 380 | ILE  | CA-C-N    | 5.51  | 125.41      | 119.85   |
| 1   | D     | 380 | ILE  | C-N-CA    | 5.51  | 125.41      | 119.85   |
| 2   | P     | 705 | GLY  | N-CA-C    | 5.50  | 118.77      | 110.18   |
| 2   | N     | 406 | ARG  | N-CA-C    | 5.49  | 119.98      | 113.28   |
| 2   | P     | 352 | LEU  | N-CA-C    | 5.49  | 118.39      | 109.06   |
| 1   | C     | 594 | TRP  | CA-CB-CG  | 5.49  | 124.03      | 113.60   |
| 1   | A     | 126 | GLU  | N-CA-C    | -5.49 | 105.30      | 111.28   |
| 2   | M     | 651 | TYR  | N-CA-C    | -5.48 | 105.41      | 111.71   |
| 2   | O     | 54  | GLY  | N-CA-C    | 5.48  | 118.01      | 110.56   |
| 1   | D     | 497 | ALA  | N-CA-C    | 5.48  | 117.59      | 108.99   |
| 2   | P     | 85  | ARG  | CG-CD-NE  | -5.47 | 99.97       | 112.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | N     | 314 | THR  | N-CA-C    | -5.46 | 105.41      | 112.68   |
| 2   | O     | 603 | ALA  | N-CA-C    | 5.46  | 117.52      | 108.13   |
| 2   | P     | 316 | ILE  | N-CA-C    | 5.45  | 120.68      | 109.34   |
| 1   | B     | 226 | ASP  | CA-C-N    | -5.44 | 113.42      | 119.19   |
| 1   | B     | 226 | ASP  | C-N-CA    | -5.44 | 113.42      | 119.19   |
| 2   | M     | 128 | LEU  | CA-C-N    | -5.44 | 114.77      | 120.38   |
| 2   | M     | 128 | LEU  | C-N-CA    | -5.44 | 114.77      | 120.38   |
| 2   | N     | 604 | ILE  | CB-CA-C   | -5.43 | 103.10      | 111.08   |
| 1   | A     | 420 | ILE  | N-CA-C    | 5.42  | 113.40      | 107.60   |
| 2   | N     | 346 | ARG  | N-CA-C    | -5.42 | 103.27      | 111.56   |
| 1   | D     | 661 | GLU  | CB-CA-C   | -5.41 | 102.39      | 110.88   |
| 1   | D     | 253 | ASP  | N-CA-C    | -5.40 | 105.48      | 111.36   |
| 2   | M     | 151 | TRP  | CA-C-N    | -5.40 | 112.62      | 120.29   |
| 2   | M     | 151 | TRP  | C-N-CA    | -5.40 | 112.62      | 120.29   |
| 1   | A     | 194 | ARG  | NE-CZ-NH2 | 5.39  | 124.06      | 119.20   |
| 2   | M     | 167 | LYS  | N-CA-C    | -5.39 | 105.06      | 111.69   |
| 2   | N     | 597 | CYS  | CA-CB-SG  | -5.39 | 102.00      | 114.40   |
| 1   | D     | 316 | CYS  | CB-CA-C   | -5.39 | 109.37      | 115.79   |
| 1   | C     | 517 | GLU  | CA-C-N    | 5.39  | 127.50      | 120.28   |
| 1   | C     | 517 | GLU  | C-N-CA    | 5.39  | 127.50      | 120.28   |
| 1   | C     | 211 | SER  | N-CA-C    | -5.38 | 105.58      | 111.82   |
| 2   | P     | 428 | LEU  | N-CA-C    | 5.37  | 117.38      | 108.20   |
| 2   | N     | 166 | SER  | N-CA-C    | 5.36  | 117.54      | 111.11   |
| 2   | O     | 604 | ILE  | N-CA-CB   | 5.35  | 117.11      | 110.05   |
| 2   | P     | 722 | ALA  | N-CA-C    | -5.33 | 105.64      | 111.82   |
| 1   | B     | 343 | THR  | N-CA-C    | -5.32 | 106.29      | 112.89   |
| 2   | M     | 677 | PHE  | N-CA-C    | -5.32 | 105.15      | 111.69   |
| 2   | N     | 408 | HIS  | CA-C-N    | 5.32  | 127.72      | 120.54   |
| 2   | N     | 408 | HIS  | C-N-CA    | 5.32  | 127.72      | 120.54   |
| 2   | M     | 57  | ASP  | CB-CA-C   | -5.31 | 104.74      | 111.86   |
| 1   | A     | 433 | LEU  | N-CA-C    | -5.31 | 105.61      | 111.71   |
| 1   | C     | 317 | CYS  | N-CA-C    | 5.30  | 117.06      | 111.28   |
| 1   | D     | 637 | ASP  | CA-C-N    | 5.30  | 125.11      | 119.28   |
| 1   | D     | 637 | ASP  | C-N-CA    | 5.30  | 125.11      | 119.28   |
| 2   | M     | 532 | SER  | N-CA-C    | -5.30 | 102.35      | 110.14   |
| 1   | D     | 539 | ILE  | N-CA-C    | 5.29  | 116.19      | 111.90   |
| 1   | A     | 553 | ASN  | N-CA-C    | -5.29 | 105.63      | 111.71   |
| 2   | M     | 693 | GLU  | CA-C-N    | -5.28 | 114.23      | 122.37   |
| 2   | M     | 693 | GLU  | C-N-CA    | -5.28 | 114.23      | 122.37   |
| 2   | P     | 242 | ASP  | N-CA-C    | 5.28  | 117.45      | 111.11   |
| 1   | B     | 588 | ALA  | N-CA-C    | -5.27 | 105.59      | 112.23   |
| 2   | N     | 400 | GLU  | N-CA-C    | -5.24 | 105.48      | 111.14   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | P     | 397 | ALA  | N-CA-C    | -5.23 | 106.20      | 112.59   |
| 2   | M     | 237 | ARG  | N-CA-C    | 5.23  | 117.39      | 111.11   |
| 2   | P     | 239 | GLU  | N-CA-C    | -5.23 | 106.16      | 112.54   |
| 2   | M     | 363 | ASP  | N-CA-C    | 5.23  | 117.81      | 110.23   |
| 1   | C     | 188 | THR  | CA-C-N    | -5.22 | 114.29      | 122.49   |
| 1   | C     | 188 | THR  | C-N-CA    | -5.22 | 114.29      | 122.49   |
| 2   | M     | 726 | ASP  | CA-C-N    | -5.22 | 114.24      | 120.13   |
| 2   | M     | 726 | ASP  | C-N-CA    | -5.22 | 114.24      | 120.13   |
| 1   | D     | 279 | VAL  | CB-CA-C   | -5.21 | 104.37      | 111.15   |
| 2   | M     | 51  | HIS  | CA-C-N    | -5.21 | 114.58      | 119.90   |
| 2   | M     | 51  | HIS  | C-N-CA    | -5.21 | 114.58      | 119.90   |
| 2   | M     | 194 | LEU  | N-CA-C    | 5.21  | 117.04      | 111.36   |
| 1   | B     | 453 | ASN  | N-CA-C    | 5.21  | 117.63      | 111.33   |
| 2   | M     | 449 | VAL  | CB-CA-C   | -5.21 | 105.03      | 111.70   |
| 2   | P     | 465 | VAL  | N-CA-C    | 5.21  | 116.16      | 108.45   |
| 2   | O     | 460 | VAL  | CA-C-N    | 5.20  | 127.67      | 120.29   |
| 2   | O     | 460 | VAL  | C-N-CA    | 5.20  | 127.67      | 120.29   |
| 2   | M     | 30  | ILE  | N-CA-C    | -5.19 | 105.44      | 110.42   |
| 2   | P     | 435 | VAL  | N-CA-C    | -5.19 | 105.48      | 110.72   |
| 1   | A     | 341 | ILE  | N-CA-C    | -5.18 | 104.61      | 111.09   |
| 1   | B     | 571 | THR  | CA-C-N    | -5.18 | 114.74      | 119.82   |
| 1   | B     | 571 | THR  | C-N-CA    | -5.18 | 114.74      | 119.82   |
| 1   | C     | 236 | ARG  | NE-CZ-NH2 | -5.18 | 114.53      | 119.20   |
| 2   | M     | 691 | LEU  | N-CA-C    | -5.18 | 105.84      | 113.61   |
| 1   | D     | 85  | GLY  | CA-C-N    | -5.18 | 113.65      | 122.56   |
| 1   | D     | 85  | GLY  | C-N-CA    | -5.18 | 113.65      | 122.56   |
| 1   | B     | 471 | ASN  | N-CA-C    | -5.18 | 101.72      | 109.95   |
| 2   | O     | 334 | ARG  | N-CA-C    | 5.17  | 118.05      | 109.46   |
| 2   | P     | 292 | PHE  | CA-C-N    | -5.17 | 113.51      | 122.10   |
| 2   | P     | 292 | PHE  | C-N-CA    | -5.17 | 113.51      | 122.10   |
| 1   | C     | 91  | GLY  | N-CA-C    | 5.17  | 122.46      | 115.32   |
| 2   | P     | 331 | GLU  | N-CA-C    | -5.17 | 101.45      | 109.72   |
| 2   | N     | 255 | LEU  | N-CA-C    | 5.16  | 117.90      | 109.59   |
| 2   | N     | 152 | THR  | CA-C-N    | -5.14 | 116.99      | 122.85   |
| 2   | N     | 152 | THR  | C-N-CA    | -5.14 | 116.99      | 122.85   |
| 2   | P     | 367 | GLU  | N-CA-C    | 5.14  | 117.44      | 108.76   |
| 2   | P     | 221 | TYR  | N-CA-C    | -5.13 | 105.14      | 111.40   |
| 1   | D     | 94  | ALA  | N-CA-C    | -5.13 | 105.69      | 111.28   |
| 2   | O     | 403 | LEU  | N-CA-C    | -5.13 | 106.72      | 112.87   |
| 1   | A     | 58  | GLN  | N-CA-C    | -5.12 | 101.92      | 110.17   |
| 1   | B     | 637 | ASP  | CA-C-N    | 5.12  | 125.16      | 119.32   |
| 1   | B     | 637 | ASP  | C-N-CA    | 5.12  | 125.16      | 119.32   |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 1   | C     | 108    | THR  | N-CA-C  | -5.12 | 105.78      | 111.36   |
| 1   | B     | 415    | ASN  | N-CA-C  | 5.12  | 118.65      | 111.90   |
| 2   | O     | 227    | MET  | N-CA-C  | -5.12 | 106.20      | 112.90   |
| 1   | D     | 595    | TRP  | N-CA-C  | -5.10 | 105.61      | 111.07   |
| 2   | M     | 166    | SER  | CB-CA-C | -5.10 | 102.32      | 110.79   |
| 2   | O     | 341    | GLU  | N-CA-C  | -5.10 | 102.23      | 110.14   |
| 2   | P     | 666    | ARG  | N-CA-C  | 5.10  | 118.76      | 112.54   |
| 2   | P     | 110    | ALA  | N-CA-C  | -5.10 | 105.80      | 111.36   |
| 1   | B     | 561    | MET  | N-CA-C  | -5.09 | 105.81      | 112.23   |
| 1   | A     | 603    | HIS  | CA-C-N  | -5.09 | 116.33      | 123.10   |
| 1   | A     | 603    | HIS  | C-N-CA  | -5.09 | 116.33      | 123.10   |
| 1   | D     | 154    | VAL  | CA-C-O  | 5.09  | 123.57      | 119.29   |
| 1   | D     | 137    | VAL  | CB-CA-C | -5.09 | 106.41      | 111.80   |
| 1   | A     | 608    | PRO  | N-CA-C  | -5.09 | 104.49      | 110.70   |
| 1   | C     | 544    | VAL  | CA-C-N  | -5.08 | 116.23      | 122.84   |
| 1   | C     | 544    | VAL  | C-N-CA  | -5.08 | 116.23      | 122.84   |
| 2   | O     | 158    | ILE  | CB-CA-C | 5.08  | 117.60      | 110.99   |
| 2   | P     | 594    | SER  | N-CA-C  | 5.06  | 117.56      | 109.81   |
| 2   | P     | 60     | TYR  | N-CA-C  | 5.06  | 118.94      | 112.26   |
| 2   | N     | 274    | PHE  | CA-C-N  | -5.05 | 115.36      | 120.31   |
| 2   | N     | 274    | PHE  | C-N-CA  | -5.05 | 115.36      | 120.31   |
| 1   | D     | 171    | LEU  | N-CA-C  | -5.05 | 105.90      | 111.71   |
| 2   | P     | 647    | ILE  | N-CA-C  | 5.05  | 117.28      | 108.90   |
| 1   | D     | 345    | ALA  | N-CA-C  | 5.04  | 119.52      | 113.17   |
| 2   | M     | 704    | ILE  | N-CA-C  | 5.04  | 116.14      | 111.81   |
| 1   | B     | 539    | ILE  | CB-CA-C | 5.03  | 119.54      | 111.29   |
| 2   | N     | 422[A] | GLN  | N-CA-C  | -5.03 | 101.10      | 108.79   |
| 2   | P     | 343    | GLY  | N-CA-C  | 5.02  | 120.24      | 112.81   |
| 1   | C     | 334    | PHE  | N-CA-C  | 5.02  | 116.44      | 110.97   |
| 1   | D     | 197    | LYS  | N-CA-C  | -5.02 | 105.70      | 111.07   |
| 2   | O     | 93     | VAL  | N-CA-CB | 5.02  | 116.72      | 111.00   |
| 1   | C     | 407    | ALA  | N-CA-C  | -5.01 | 106.01      | 111.82   |
| 1   | A     | 363    | VAL  | N-CA-C  | -5.00 | 105.72      | 110.42   |
| 2   | M     | 221    | TYR  | N-CA-C  | -5.00 | 104.78      | 111.24   |
| 2   | M     | 441    | PHE  | N-CA-C  | 5.00  | 118.16      | 111.75   |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 414 | SER  | Peptide |
| 1   | B     | 469 | GLY  | Peptide |

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| Mol | Chain | Res    | Type | Group   |
|-----|-------|--------|------|---------|
| 1   | C     | 415    | ASN  | Peptide |
| 1   | C     | 469    | GLY  | Peptide |
| 1   | D     | 469    | GLY  | Peptide |
| 2   | N     | 313    | LEU  | Peptide |
| 2   | P     | 315[A] | LYS  | Peptide |
| 2   | P     | 389    | ASP  | Peptide |

## 5.2 Too-close contacts [i](#)

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     | 5094  | 0        | 5088     | 124     | 0            |
| 1   | B     | 5094  | 0        | 5082     | 142     | 0            |
| 1   | C     | 5094  | 0        | 5086     | 143     | 0            |
| 1   | D     | 5094  | 0        | 5093     | 162     | 0            |
| 2   | M     | 5740  | 0        | 5693     | 116     | 0            |
| 2   | N     | 5740  | 0        | 5695     | 136     | 0            |
| 2   | O     | 5725  | 0        | 5680     | 329     | 0            |
| 2   | P     | 5740  | 0        | 5693     | 259     | 0            |
| 3   | A     | 16    | 0        | 0        | 0       | 0            |
| 3   | B     | 8     | 0        | 0        | 1       | 0            |
| 3   | C     | 16    | 0        | 0        | 0       | 0            |
| 3   | D     | 8     | 0        | 0        | 0       | 0            |
| 3   | M     | 8     | 0        | 0        | 0       | 0            |
| 3   | N     | 8     | 0        | 0        | 0       | 0            |
| 3   | O     | 8     | 0        | 0        | 5       | 0            |
| 3   | P     | 8     | 0        | 0        | 1       | 0            |
| 4   | A     | 9     | 0        | 0        | 2       | 0            |
| 4   | B     | 9     | 0        | 0        | 3       | 0            |
| 4   | C     | 9     | 0        | 0        | 3       | 0            |
| 4   | D     | 9     | 0        | 0        | 1       | 0            |
| 5   | A     | 7     | 0        | 0        | 11      | 0            |
| 5   | B     | 7     | 0        | 0        | 12      | 0            |
| 5   | C     | 7     | 0        | 0        | 7       | 0            |
| 5   | D     | 7     | 0        | 0        | 6       | 0            |
| 5   | M     | 3     | 0        | 0        | 2       | 0            |
| 5   | N     | 4     | 0        | 0        | 5       | 0            |
| 5   | O     | 3     | 0        | 0        | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | P     | 4     | 0        | 0        | 4       | 0            |
| 6   | A     | 24    | 0        | 32       | 5       | 0            |
| 6   | B     | 18    | 0        | 24       | 5       | 0            |
| 6   | C     | 12    | 0        | 16       | 1       | 0            |
| 6   | D     | 12    | 0        | 16       | 7       | 0            |
| 7   | M     | 1     | 0        | 0        | 0       | 0            |
| 7   | N     | 1     | 0        | 0        | 0       | 0            |
| 7   | O     | 1     | 0        | 0        | 1       | 0            |
| 7   | P     | 1     | 0        | 0        | 0       | 0            |
| 8   | M     | 1     | 0        | 0        | 0       | 0            |
| 8   | N     | 1     | 0        | 0        | 0       | 0            |
| 8   | O     | 1     | 0        | 0        | 0       | 0            |
| 8   | P     | 1     | 0        | 0        | 0       | 0            |
| 9   | A     | 168   | 0        | 0        | 5       | 0            |
| 9   | B     | 220   | 0        | 0        | 13      | 0            |
| 9   | C     | 130   | 0        | 0        | 14      | 0            |
| 9   | D     | 105   | 0        | 0        | 12      | 0            |
| 9   | M     | 201   | 0        | 0        | 9       | 0            |
| 9   | N     | 222   | 0        | 0        | 20      | 0            |
| 9   | O     | 27    | 0        | 0        | 5       | 0            |
| 9   | P     | 80    | 0        | 0        | 8       | 0            |
| All | All   | 44706 | 0        | 43198    | 1373    | 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 (1373) 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:114[A]:CYS:HB2 | 9:B:1217:HOH:O   | 1.29                     | 1.28              |
| 2:O:373:ILE:HG22   | 2:O:440:ARG:HG3  | 1.28                     | 1.09              |
| 2:P:602:MET:HE1    | 2:P:645:MET:HE2  | 1.32                     | 1.09              |
| 1:B:148[A]:ARG:NH1 | 9:B:1185:HOH:O   | 1.78                     | 1.08              |
| 1:D:114:CYS:HB2    | 9:D:1050:HOH:O   | 1.50                     | 1.08              |
| 1:D:279:VAL:HG11   | 1:D:315:ILE:HD12 | 1.34                     | 1.07              |
| 1:D:105:MET:CE     | 1:D:609:PRO:HD3  | 1.84                     | 1.06              |
| 1:D:525:LYS:HE2    | 9:D:1094:HOH:O   | 1.57                     | 1.04              |
| 1:D:105:MET:HE2    | 1:D:609:PRO:CD   | 1.93                     | 0.99              |
| 1:A:577:VAL:HG21   | 1:A:645:ILE:HG23 | 1.41                     | 0.98              |
| 2:O:144:PHE:O      | 2:O:148:MET:HG3  | 1.64                     | 0.98              |
| 6:A:862:GOL:H31    | 2:M:259:ASP:HB3  | 1.44                     | 0.97              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:O:698:LYS:HA    | 2:O:718:LYS:HG2   | 1.46                     | 0.96              |
| 2:M:602:MET:HE2   | 2:M:647:ILE:HD13  | 1.48                     | 0.96              |
| 2:O:670:MET:HG2   | 2:O:674:LEU:HD23  | 1.48                     | 0.95              |
| 2:N:588:MET:HE1   | 2:N:604:ILE:HG23  | 1.48                     | 0.95              |
| 1:C:587:LYS:H     | 1:D:220:HIS:HE1   | 1.13                     | 0.95              |
| 1:D:105:MET:HE2   | 1:D:609:PRO:HD3   | 1.50                     | 0.94              |
| 2:P:354:ARG:HH21  | 2:P:356:VAL:CG1   | 1.80                     | 0.94              |
| 2:P:384:LEU:HA    | 2:P:468:PHE:O     | 1.66                     | 0.94              |
| 2:N:722:ALA:HA    | 2:N:725:MET:HE3   | 1.50                     | 0.93              |
| 2:O:363:ASP:HB2   | 2:O:462:ARG:HD2   | 1.52                     | 0.92              |
| 1:D:279:VAL:HG11  | 1:D:315:ILE:CD1   | 2.00                     | 0.91              |
| 1:B:577:VAL:HG21  | 1:B:645:ILE:HG23  | 1.53                     | 0.90              |
| 1:B:110:ALA:O     | 1:B:114[A]:CYS:SG | 2.30                     | 0.89              |
| 2:O:334:ARG:HG3   | 9:O:1028:HOH:O    | 1.74                     | 0.88              |
| 2:O:508:LEU:HB3   | 3:O:900:SF4:S1    | 2.14                     | 0.88              |
| 2:P:490:ASP:C     | 2:P:492:MET:H     | 1.80                     | 0.87              |
| 1:C:620:LEU:HD23  | 5:C:1004:XE:XE    | 2.52                     | 0.87              |
| 7:O:950:CU1:CU    | 5:O:1009:XE:XE    | 2.02                     | 0.87              |
| 1:A:114:CYS:HB2   | 9:A:1134:HOH:O    | 1.73                     | 0.86              |
| 2:P:187:ASP:HA    | 2:P:211:ASN:HD22  | 1.39                     | 0.86              |
| 2:P:588:MET:HE1   | 2:P:604:ILE:HD13  | 1.57                     | 0.86              |
| 2:M:621:MET:HE1   | 2:M:625:GLY:HA2   | 1.55                     | 0.86              |
| 2:O:407:ILE:HG23  | 2:O:408:HIS:H     | 1.40                     | 0.86              |
| 1:D:335:ALA:H     | 1:D:471:ASN:HD22  | 1.19                     | 0.85              |
| 2:N:163:ALA:H     | 2:N:192:GLN:HE22  | 1.25                     | 0.85              |
| 1:C:114:CYS:HB2   | 9:C:1089:HOH:O    | 1.75                     | 0.85              |
| 6:B:863:GOL:H32   | 2:N:27:HIS:CE1    | 2.12                     | 0.85              |
| 1:A:105:MET:HE1   | 1:B:72:MET:HG3    | 1.59                     | 0.85              |
| 1:C:126:GLU:OE1   | 1:C:390:THR:OG1   | 1.93                     | 0.84              |
| 2:O:187:ASP:HA    | 2:O:211:ASN:HD22  | 1.40                     | 0.84              |
| 2:O:373:ILE:HG22  | 2:O:440:ARG:CG    | 2.08                     | 0.84              |
| 1:A:105:MET:HE1   | 1:B:72:MET:CG     | 2.08                     | 0.83              |
| 1:B:400:ALA:HA    | 1:B:403:MET:CE    | 2.08                     | 0.83              |
| 2:P:549:GLN:HG3   | 2:P:550:PRO:HD2   | 1.57                     | 0.83              |
| 2:M:696:ILE:HA    | 2:M:699:ILE:HD12  | 1.61                     | 0.82              |
| 1:D:102:VAL:HG13  | 5:D:1003[B]:XE:XE | 2.57                     | 0.82              |
| 2:M:621:MET:HE1   | 2:M:625:GLY:CA    | 2.10                     | 0.82              |
| 2:P:95:ASN:C      | 2:P:95:ASN:HD22   | 1.86                     | 0.82              |
| 1:D:105:MET:CE    | 1:D:609:PRO:CD    | 2.56                     | 0.81              |
| 2:P:522:PRO:HD3   | 2:P:533:TRP:CD1   | 2.15                     | 0.81              |
| 1:B:114[A]:CYS:SG | 9:B:1161:HOH:O    | 2.38                     | 0.81              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:114:CYS:SG   | 1:C:209:HIS:CD2   | 2.73                     | 0.81              |
| 2:P:602:MET:HE1  | 2:P:645:MET:CE    | 2.10                     | 0.80              |
| 2:O:371:PRO:HD2  | 2:O:469:THR:HB    | 1.63                     | 0.79              |
| 2:O:468:PHE:HB2  | 2:O:474:VAL:HG23  | 1.63                     | 0.79              |
| 1:C:620:LEU:HD21 | 5:C:1003[A]:XE:XE | 2.61                     | 0.79              |
| 1:D:470:CYS:HB3  | 4:D:800:XCC:S2    | 2.23                     | 0.79              |
| 1:C:102:VAL:CG1  | 5:C:1003[B]:XE:XE | 3.09                     | 0.79              |
| 2:O:373:ILE:CG2  | 2:O:440:ARG:HG3   | 2.12                     | 0.78              |
| 2:O:411:ILE:HD13 | 2:O:428:LEU:HD21  | 1.64                     | 0.78              |
| 2:P:343:GLY:HA3  | 2:P:349:ALA:HB3   | 1.66                     | 0.78              |
| 1:D:559:LEU:HG   | 1:D:563:MET:HE3   | 1.64                     | 0.78              |
| 2:O:612:MET:SD   | 2:O:624:SER:HB3   | 2.24                     | 0.78              |
| 1:C:411:ARG:HG3  | 1:C:416:ARG:HD3   | 1.64                     | 0.78              |
| 2:M:451:LYS:NZ   | 2:M:454:GLU:OE1   | 2.14                     | 0.77              |
| 2:O:396:GLN:HB2  | 2:O:399:PHE:CE2   | 2.18                     | 0.77              |
| 1:C:114:CYS:SG   | 1:C:209:HIS:NE2   | 2.58                     | 0.77              |
| 2:P:588:MET:CE   | 2:P:604:ILE:HD13  | 2.15                     | 0.77              |
| 1:D:614:ASP:N    | 6:D:863:GOL:H11   | 2.00                     | 0.77              |
| 2:M:163:ALA:H    | 2:M:192:GLN:HE22  | 1.33                     | 0.76              |
| 1:C:563:MET:CE   | 1:C:576:PHE:HD2   | 1.97                     | 0.76              |
| 2:N:187:ASP:HA   | 2:N:211:ASN:HD22  | 1.50                     | 0.76              |
| 2:O:6:LYS:HA     | 2:O:9:GLU:HG3     | 1.67                     | 0.76              |
| 1:A:335:ALA:H    | 1:A:471:ASN:HD22  | 1.31                     | 0.76              |
| 1:B:580:ALA:HB2  | 5:B:1001:XE:XE    | 2.62                     | 0.76              |
| 2:P:602:MET:HE3  | 2:P:645:MET:HB3   | 1.68                     | 0.76              |
| 1:A:294:ALA:O    | 1:A:298:MET:HG3   | 1.86                     | 0.75              |
| 2:P:156:GLU:HG2  | 5:P:1008:XE:XE    | 2.64                     | 0.75              |
| 1:A:622:GLN:HB3  | 6:A:862:GOL:H11   | 1.67                     | 0.75              |
| 2:M:640:GLN:HB2  | 9:M:1157:HOH:O    | 1.85                     | 0.75              |
| 2:P:525:VAL:HG11 | 2:P:650:THR:CG2   | 2.15                     | 0.75              |
| 1:C:470:CYS:HB3  | 4:C:800:XCC:S2    | 2.27                     | 0.75              |
| 2:P:572:TYR:CE2  | 2:P:577:ARG:HG2   | 2.22                     | 0.75              |
| 2:O:407:ILE:CG2  | 2:O:408:HIS:H     | 1.98                     | 0.74              |
| 2:O:14:GLU:HA    | 9:O:1027:HOH:O    | 1.86                     | 0.74              |
| 2:O:333:ILE:HG21 | 2:O:429:ARG:HB3   | 1.69                     | 0.74              |
| 2:P:555:GLY:HA3  | 2:P:565:LYS:HB3   | 1.69                     | 0.74              |
| 2:O:406:ARG:O    | 2:O:410:PHE:CD2   | 2.41                     | 0.74              |
| 1:A:577:VAL:HG21 | 1:A:645:ILE:CG2   | 2.18                     | 0.74              |
| 1:D:280:LEU:HD13 | 1:D:288:SER:HB2   | 1.69                     | 0.74              |
| 1:C:105:MET:HE1  | 1:C:609:PRO:HD3   | 1.68                     | 0.73              |
| 1:D:302:ALA:O    | 1:D:307:ALA:HB3   | 1.89                     | 0.73              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:279:VAL:CG1  | 1:D:315:ILE:HD12  | 2.16                     | 0.73              |
| 1:D:460:GLU:OE1  | 1:D:530:ARG:NH2   | 2.22                     | 0.73              |
| 2:P:381:LYS:O    | 2:P:382:LEU:HD13  | 1.87                     | 0.73              |
| 1:D:525:LYS:CE   | 9:D:1094:HOH:O    | 2.25                     | 0.73              |
| 2:N:588:MET:HE3  | 2:N:728:ILE:HG12  | 1.70                     | 0.73              |
| 2:P:568:ASN:HD21 | 2:P:581:GLN:HG3   | 1.52                     | 0.73              |
| 1:B:400:ALA:HA   | 1:B:403:MET:HE3   | 1.69                     | 0.73              |
| 1:A:68:CYS:HB2   | 1:A:97:ILE:HG23   | 1.71                     | 0.73              |
| 1:A:33:VAL:HG21  | 1:A:477:GLN:HE22  | 1.54                     | 0.72              |
| 2:M:344:GLY:O    | 2:M:345:ASN:HB2   | 1.88                     | 0.72              |
| 2:O:469:THR:O    | 2:O:470:ASP:HB2   | 1.88                     | 0.72              |
| 1:C:51:ARG:HD3   | 9:C:1137:HOH:O    | 1.89                     | 0.72              |
| 2:M:3:ASP:CG     | 9:M:1198:HOH:O    | 2.32                     | 0.72              |
| 2:O:418:TRP:O    | 2:O:428:LEU:HA    | 1.90                     | 0.72              |
| 2:P:163:ALA:H    | 2:P:192:GLN:HE22  | 1.38                     | 0.72              |
| 2:M:189:ALA:HA   | 2:M:192:GLN:HE21  | 1.53                     | 0.72              |
| 1:D:32:ALA:HB1   | 1:D:268:MET:HG3   | 1.72                     | 0.72              |
| 2:N:229:PHE:CD1  | 5:N:1009:XE:XE    | 3.21                     | 0.71              |
| 2:O:407:ILE:HG23 | 2:O:408:HIS:N     | 2.05                     | 0.71              |
| 2:P:95:ASN:ND2   | 2:P:98:ASN:H      | 1.87                     | 0.71              |
| 1:D:114:CYS:SG   | 1:D:209:HIS:CD2   | 2.83                     | 0.71              |
| 2:P:354:ARG:HH21 | 2:P:356:VAL:HG13  | 1.54                     | 0.71              |
| 1:D:614:ASP:H    | 6:D:863:GOL:H11   | 1.55                     | 0.71              |
| 1:C:102:VAL:HG13 | 5:C:1003[B]:XE:XE | 2.69                     | 0.71              |
| 2:O:361:ILE:HD13 | 2:O:391:TYR:HB2   | 1.73                     | 0.71              |
| 2:P:383:PRO:HB2  | 2:P:474:VAL:HG21  | 1.73                     | 0.71              |
| 2:P:560:ILE:O    | 2:P:660:ALA:HB2   | 1.90                     | 0.71              |
| 1:B:77:ARG:HD3   | 9:B:1199:HOH:O    | 1.90                     | 0.71              |
| 1:C:620:LEU:CD2  | 5:C:1004:XE:XE    | 3.17                     | 0.70              |
| 2:M:408:HIS:HD2  | 2:M:419:HIS:ND1   | 1.90                     | 0.70              |
| 2:O:181:PHE:HE2  | 2:O:306:MET:HE3   | 1.56                     | 0.70              |
| 2:P:568:ASN:ND2  | 2:P:581:GLN:HA    | 2.07                     | 0.70              |
| 2:N:150:ASP:OD1  | 2:N:152:THR:HG23  | 1.92                     | 0.70              |
| 2:O:341:GLU:OE2  | 2:O:343:GLY:N     | 2.22                     | 0.70              |
| 2:O:346:ARG:HB2  | 2:O:346:ARG:HH11  | 1.56                     | 0.70              |
| 2:O:429:ARG:N    | 9:O:1018:HOH:O    | 2.25                     | 0.70              |
| 1:D:364:ALA:HB1  | 1:D:369:THR:HB    | 1.74                     | 0.70              |
| 2:O:62:LEU:HD12  | 2:O:65:ILE:HD12   | 1.72                     | 0.70              |
| 2:O:580:GLU:O    | 2:O:581:GLN:HB2   | 1.90                     | 0.70              |
| 1:C:577:VAL:HG21 | 1:C:645:ILE:HG23  | 1.73                     | 0.69              |
| 2:M:150:ASP:OD1  | 2:M:152:THR:HG23  | 1.92                     | 0.69              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 1:C:416:ARG:HD2  | 1:C:418:VAL:HG23    | 1.74                     | 0.69              |
| 2:N:588:MET:CE   | 2:N:728:ILE:HG12    | 2.21                     | 0.69              |
| 2:P:150:ASP:OD1  | 2:P:152:THR:HG23    | 1.92                     | 0.69              |
| 1:C:283:HIS:CD2  | 1:C:317:CYS:HB2     | 2.26                     | 0.69              |
| 1:D:102:VAL:CG1  | 5:D:1003[B]:XE:XE   | 3.19                     | 0.69              |
| 1:D:65:GLY:HA2   | 9:D:1089:HOH:O      | 1.92                     | 0.69              |
| 2:N:588:MET:HE1  | 2:N:604:ILE:CG2     | 2.22                     | 0.69              |
| 2:N:261:VAL:HG12 | 5:N:1006:XE:XE      | 2.70                     | 0.69              |
| 1:A:24:ASN:O     | 1:A:27:ARG:HG2      | 1.93                     | 0.69              |
| 1:B:470:CYS:HB3  | 4:B:800:XCC:S2      | 2.32                     | 0.69              |
| 2:O:252:VAL:HB   | 2:O:276:VAL:HG22    | 1.74                     | 0.69              |
| 2:O:509:CYS:SG   | 2:O:595:CYS:SG      | 2.91                     | 0.69              |
| 1:C:482:LEU:HD13 | 1:C:486:LYS:HD2     | 1.75                     | 0.69              |
| 1:B:577:VAL:HG21 | 1:B:645:ILE:CG2     | 2.23                     | 0.68              |
| 2:P:490:ASP:C    | 2:P:492:MET:N       | 2.50                     | 0.68              |
| 1:B:416:ARG:HG3  | 1:B:416:ARG:HH11    | 1.56                     | 0.68              |
| 1:C:78:ILE:HD11  | 1:C:97:ILE:HD12     | 1.75                     | 0.68              |
| 2:M:415:GLU:OE1  | 9:M:1206:HOH:O      | 2.11                     | 0.68              |
| 2:O:491:ARG:HB2  | 2:O:491:ARG:HH11    | 1.58                     | 0.68              |
| 2:O:675:LYS:HA   | 2:O:696:ILE:HD11    | 1.75                     | 0.68              |
| 2:P:342:MET:HG3  | 2:P:384:LEU:HD22    | 1.75                     | 0.68              |
| 1:A:2:PRO:N      | 6:A:862:GOL:HO1     | 1.92                     | 0.67              |
| 2:M:445:GLY:HA2  | 2:M:465:VAL:HG11    | 1.76                     | 0.67              |
| 1:C:12:ARG:O     | 6:C:861:GOL:H12     | 1.94                     | 0.67              |
| 2:O:649:ARG:O    | 2:O:652:ILE:HD12    | 1.94                     | 0.67              |
| 2:O:96:PHE:O     | 2:O:100:ARG:HG3     | 1.95                     | 0.67              |
| 2:P:474:VAL:CG1  | 2:P:475:LYS:N       | 2.58                     | 0.67              |
| 1:B:510:LEU:N    | 1:B:510:LEU:HD12    | 2.08                     | 0.67              |
| 2:M:373:ILE:CG2  | 2:M:440:ARG:HD3     | 2.25                     | 0.66              |
| 1:B:63:TYR:OH    | 9:B:1210:HOH:O      | 2.13                     | 0.66              |
| 2:P:338:MET:SD   | 2:P:341:GLU:HB2     | 2.35                     | 0.66              |
| 1:A:280:LEU:HD13 | 1:A:288:SER:HB2     | 1.77                     | 0.66              |
| 1:B:468:CYS:SG   | 5:B:1001:XE:XE      | 3.32                     | 0.66              |
| 2:N:354:ARG:HD2  | 2:N:389:ASP:OD1     | 1.95                     | 0.66              |
| 2:O:63:PRO:HB2   | 2:O:220:ASN:HB2     | 1.78                     | 0.66              |
| 2:O:488:ARG:C    | 2:O:490:ASP:H       | 2.02                     | 0.66              |
| 2:P:143:ARG:O    | 2:P:146[A]:ILE:HD13 | 1.95                     | 0.66              |
| 2:P:602:MET:CE   | 2:P:645:MET:HE2     | 2.19                     | 0.66              |
| 1:A:105:MET:CE   | 1:B:72:MET:HG3      | 2.25                     | 0.66              |
| 1:C:159:VAL:HG13 | 9:C:1052:HOH:O      | 1.95                     | 0.66              |
| 2:O:516:HIS:CD2  | 2:O:593:THR:OG1     | 2.49                     | 0.66              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:217:ASN:ND2  | 1:D:112:ALA:HA    | 2.10                     | 0.66              |
| 1:C:563:MET:HE2  | 1:C:576:PHE:HD2   | 1.61                     | 0.66              |
| 1:D:470:CYS:O    | 1:D:582:GLU:HB2   | 1.94                     | 0.66              |
| 2:O:649:ARG:HA   | 2:O:652:ILE:CD1   | 2.26                     | 0.66              |
| 2:N:315:LYS:HD3  | 9:N:1162:HOH:O    | 1.95                     | 0.65              |
| 2:O:524:ARG:NH1  | 2:O:645:MET:HE3   | 2.11                     | 0.65              |
| 2:P:474:VAL:CG1  | 2:P:475:LYS:H     | 2.10                     | 0.65              |
| 2:P:316:ILE:HG23 | 2:P:316:ILE:O     | 1.96                     | 0.65              |
| 1:B:400:ALA:HB2  | 5:B:1010:XE:XE    | 2.75                     | 0.65              |
| 1:C:442:THR:HG21 | 1:C:537:ILE:HD11  | 1.79                     | 0.65              |
| 2:M:428:LEU:N    | 2:M:428:LEU:HD12  | 2.11                     | 0.65              |
| 2:P:387:LEU:O    | 2:P:465:VAL:HA    | 1.96                     | 0.65              |
| 1:C:587:LYS:H    | 1:D:220:HIS:CE1   | 2.05                     | 0.65              |
| 2:O:556:GLU:HG2  | 2:O:557:ILE:N     | 2.12                     | 0.65              |
| 1:B:372:ILE:HD13 | 1:B:403:MET:HE3   | 1.77                     | 0.65              |
| 2:M:617:ASP:HB2  | 9:M:1199:HOH:O    | 1.97                     | 0.65              |
| 2:M:15:GLY:O     | 2:M:16:LYS:HD3    | 1.97                     | 0.65              |
| 2:N:722:ALA:HA   | 2:N:725:MET:CE    | 2.26                     | 0.65              |
| 2:O:374:ASP:HB2  | 2:O:440:ARG:HE    | 1.62                     | 0.65              |
| 2:O:316:ILE:HG23 | 2:O:316:ILE:O     | 1.96                     | 0.65              |
| 2:P:189:ALA:HA   | 2:P:192:GLN:HE21  | 1.62                     | 0.65              |
| 1:C:2:PRO:N      | 1:C:625:SER:HG    | 1.95                     | 0.64              |
| 1:D:105:MET:HE2  | 1:D:609:PRO:CG    | 2.28                     | 0.64              |
| 1:A:102:VAL:CG1  | 5:A:1003[B]:XE:XE | 3.24                     | 0.64              |
| 1:A:220:HIS:HE1  | 1:B:587:LYS:H     | 1.43                     | 0.64              |
| 2:N:146:ILE:O    | 2:N:146:ILE:HG13  | 1.96                     | 0.64              |
| 2:O:568:ASN:ND2  | 2:O:581:GLN:HG2   | 2.12                     | 0.64              |
| 2:O:346:ARG:HB2  | 2:O:346:ARG:NH1   | 2.12                     | 0.64              |
| 2:O:181:PHE:CE2  | 2:O:306:MET:HE3   | 2.33                     | 0.64              |
| 2:P:489:ASP:HA   | 2:P:492:MET:HB2   | 1.79                     | 0.64              |
| 1:B:287:LEU:CD1  | 1:B:388:TYR:CE1   | 2.81                     | 0.64              |
| 1:C:640:VAL:HG12 | 1:C:644:LYS:HE3   | 1.80                     | 0.64              |
| 2:O:351:GLU:HA   | 2:O:386:ILE:HB    | 1.79                     | 0.64              |
| 1:B:316:CYS:H    | 1:B:503:GLN:HE22  | 1.45                     | 0.64              |
| 2:O:556:GLU:HG2  | 2:O:557:ILE:H     | 1.63                     | 0.64              |
| 2:O:580:GLU:O    | 2:O:581:GLN:CB    | 2.46                     | 0.64              |
| 2:O:334:ARG:HH11 | 2:O:335:LYS:HG3   | 1.63                     | 0.63              |
| 2:P:588:MET:HE1  | 2:P:604:ILE:CD1   | 2.27                     | 0.63              |
| 2:O:2:THR:HA     | 2:O:5:ASP:HB2     | 1.81                     | 0.63              |
| 1:C:30:ASP:OD2   | 1:C:507:LYS:NZ    | 2.30                     | 0.63              |
| 1:D:500:CYS:HA   | 1:D:503:GLN:HG3   | 1.79                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:P:666:ARG:HD2  | 2:P:728:ILE:HD13  | 1.80                     | 0.63              |
| 1:A:357:MET:HG2  | 1:B:90:CYS:O      | 1.98                     | 0.63              |
| 1:C:335:ALA:H    | 1:C:471:ASN:HD22  | 1.45                     | 0.63              |
| 1:D:416:ARG:HB2  | 1:D:418:VAL:HG23  | 1.80                     | 0.63              |
| 2:M:95:ASN:ND2   | 2:M:98:ASN:H      | 1.95                     | 0.63              |
| 2:O:157:ALA:HB3  | 2:O:183:LEU:CD2   | 2.29                     | 0.63              |
| 2:P:95:ASN:HD21  | 2:P:98:ASN:H      | 1.46                     | 0.63              |
| 2:P:522:PRO:HD3  | 2:P:533:TRP:CG    | 2.34                     | 0.63              |
| 2:O:584:LEU:HD23 | 2:O:592:MET:HE1   | 1.80                     | 0.63              |
| 1:A:15:GLU:OE2   | 6:A:861:GOL:H12   | 1.99                     | 0.63              |
| 2:P:474:VAL:HG13 | 2:P:475:LYS:N     | 2.14                     | 0.62              |
| 1:C:316:CYS:H    | 1:C:503:GLN:HE22  | 1.47                     | 0.62              |
| 1:D:18:ARG:CD    | 1:D:636:MET:HE3   | 2.30                     | 0.62              |
| 1:C:615:LEU:O    | 1:C:615:LEU:HD23  | 1.99                     | 0.62              |
| 1:D:658:VAL:O    | 1:D:662:VAL:HG23  | 1.99                     | 0.62              |
| 2:M:498:GLU:OE2  | 2:M:656:LYS:NZ    | 2.27                     | 0.62              |
| 2:O:556:GLU:HA   | 2:O:564:TRP:CD1   | 2.35                     | 0.62              |
| 2:N:396:GLN:NE2  | 9:N:1215:HOH:O    | 2.30                     | 0.62              |
| 2:O:384:LEU:HD12 | 2:O:385:GLY:H     | 1.65                     | 0.62              |
| 6:B:863:GOL:H32  | 2:N:27:HIS:HE1    | 1.62                     | 0.62              |
| 2:O:556:GLU:HA   | 2:O:564:TRP:HD1   | 1.63                     | 0.62              |
| 1:B:281:HIS:HB3  | 1:B:351:VAL:HG12  | 1.82                     | 0.62              |
| 2:O:149:VAL:HG11 | 2:O:509:CYS:HA    | 1.81                     | 0.62              |
| 2:O:333:ILE:HG21 | 2:O:429:ARG:CB    | 2.30                     | 0.62              |
| 2:P:605:LEU:HD21 | 2:P:623:PRO:HB2   | 1.80                     | 0.62              |
| 1:B:335:ALA:H    | 1:B:471:ASN:HD22  | 1.46                     | 0.62              |
| 2:O:346:ARG:HG3  | 2:O:381:LYS:NZ    | 2.15                     | 0.62              |
| 1:C:11:CYS:HB2   | 1:C:621:THR:HB    | 1.83                     | 0.61              |
| 1:D:182:GLU:HG2  | 1:D:204:VAL:HG11  | 1.82                     | 0.61              |
| 1:C:12:ARG:HD3   | 9:C:1107:HOH:O    | 1.99                     | 0.61              |
| 2:M:587:LEU:HD23 | 2:M:588:MET:HE2   | 1.82                     | 0.61              |
| 2:N:373:ILE:HD12 | 2:N:441:PHE:CZ    | 2.35                     | 0.61              |
| 2:O:221:TYR:CA   | 2:O:224:ARG:HH21  | 2.13                     | 0.61              |
| 2:O:431:SER:O    | 2:O:434:ALA:N     | 2.24                     | 0.61              |
| 1:A:7:LEU:HD11   | 2:M:164:LYS:HB2   | 1.83                     | 0.61              |
| 2:P:187:ASP:HA   | 2:P:211:ASN:ND2   | 2.15                     | 0.61              |
| 2:N:156:GLU:HG3  | 2:N:182:MET:HB3   | 1.82                     | 0.61              |
| 2:O:221:TYR:HA   | 2:O:224:ARG:HH21  | 1.66                     | 0.61              |
| 2:P:174:LYS:HE2  | 2:P:323:ASN:OD1   | 2.00                     | 0.61              |
| 1:B:102:VAL:HG13 | 5:B:1003[B]:XE:XE | 2.79                     | 0.61              |
| 1:D:272:ASP:OD2  | 1:D:275:GLN:NE2   | 2.33                     | 0.61              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:O:468:PHE:CB     | 2:O:474:VAL:HG23  | 2.31                     | 0.61              |
| 2:P:164:LYS:NZ     | 9:P:1089:HOH:O    | 2.34                     | 0.61              |
| 2:N:728:ILE:O      | 2:N:729:MET:HB2   | 1.98                     | 0.61              |
| 2:P:611:ILE:O      | 2:P:611:ILE:HG13  | 2.01                     | 0.61              |
| 2:M:657:PHE:O      | 2:M:658:ILE:C     | 2.44                     | 0.60              |
| 2:N:300:LYS:HD2    | 9:N:1202:HOH:O    | 2.01                     | 0.60              |
| 2:O:698:LYS:HA     | 2:O:718:LYS:CG    | 2.27                     | 0.60              |
| 1:A:559:LEU:HG     | 1:A:563:MET:CE    | 2.31                     | 0.60              |
| 2:P:681:GLU:HG3    | 2:P:684:ARG:HH21  | 1.64                     | 0.60              |
| 1:B:220:HIS:HD2    | 1:B:221:MET:O     | 1.85                     | 0.60              |
| 1:C:273:PRO:HD3    | 1:C:420:ILE:HD12  | 1.83                     | 0.60              |
| 2:M:585:TYR:CZ     | 2:M:656:LYS:HE3   | 2.36                     | 0.60              |
| 2:P:354:ARG:NH2    | 2:P:356:VAL:CG1   | 2.59                     | 0.60              |
| 1:B:287:LEU:HD13   | 1:B:388:TYR:CE1   | 2.37                     | 0.60              |
| 2:O:334:ARG:HH11   | 2:O:335:LYS:CG    | 2.14                     | 0.60              |
| 2:O:549:GLN:HB3    | 2:O:550:PRO:HD2   | 1.83                     | 0.60              |
| 2:O:560:ILE:O      | 2:O:660:ALA:HB2   | 2.01                     | 0.60              |
| 2:P:342:MET:CG     | 2:P:384:LEU:HD22  | 2.31                     | 0.60              |
| 1:B:114[A]:CYS:CB  | 9:B:1161:HOH:O    | 2.50                     | 0.60              |
| 2:O:623:PRO:HB3    | 2:O:707:THR:C     | 2.25                     | 0.60              |
| 2:P:672:LYS:HE3    | 2:P:676:ASP:OD2   | 2.01                     | 0.60              |
| 1:C:7:LEU:HD11     | 2:O:164:LYS:HB2   | 1.84                     | 0.60              |
| 2:M:587:LEU:HD23   | 2:M:588:MET:CE    | 2.32                     | 0.60              |
| 2:O:346:ARG:HG3    | 2:O:381:LYS:HZ3   | 1.67                     | 0.60              |
| 1:A:18:ARG:NE      | 1:A:636:MET:HE3   | 2.17                     | 0.60              |
| 1:A:602:THR:CG2    | 5:A:1001:XE:XE    | 3.28                     | 0.60              |
| 1:B:114[A]:CYS:HB3 | 9:B:1161:HOH:O    | 2.01                     | 0.60              |
| 1:B:325:ARG:HD2    | 9:B:1067:HOH:O    | 2.02                     | 0.60              |
| 2:N:124:ASP:OD2    | 2:N:125:GLU:HB2   | 2.02                     | 0.60              |
| 2:N:163:ALA:N      | 2:N:192:GLN:HE22  | 1.96                     | 0.60              |
| 1:A:112:ALA:HA     | 1:B:217:ASN:HD22  | 1.67                     | 0.59              |
| 2:O:175:GLU:HG2    | 2:O:179:MET:HE2   | 1.83                     | 0.59              |
| 2:P:523:GLU:O      | 2:P:654:SER:OG    | 2.17                     | 0.59              |
| 1:A:102:VAL:HG13   | 5:A:1003[B]:XE:XE | 2.80                     | 0.59              |
| 1:B:400:ALA:HA     | 1:B:403:MET:HE2   | 1.81                     | 0.59              |
| 1:D:114:CYS:SG     | 1:D:209:HIS:NE2   | 2.74                     | 0.59              |
| 1:D:281:HIS:HB3    | 1:D:351:VAL:HG12  | 1.84                     | 0.59              |
| 2:M:424:ASN:HD22   | 2:M:424:ASN:H     | 1.48                     | 0.59              |
| 2:P:391:TYR:HD2    | 2:P:462:ARG:NH1   | 2.00                     | 0.59              |
| 1:A:615:LEU:C      | 1:A:615:LEU:HD23  | 2.27                     | 0.59              |
| 1:C:294:ALA:O      | 1:C:298:MET:HG2   | 2.00                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:O:221:TYR:HA   | 2:O:224:ARG:NH2   | 2.18                     | 0.59              |
| 2:O:429:ARG:HG3  | 9:O:1018:HOH:O    | 2.02                     | 0.59              |
| 2:P:389:ASP:O    | 2:P:463:VAL:HA    | 2.01                     | 0.59              |
| 2:P:525:VAL:HG11 | 2:P:650:THR:HG23  | 1.83                     | 0.59              |
| 2:N:602:MET:HE2  | 2:N:647:ILE:HD13  | 1.82                     | 0.59              |
| 2:O:407:ILE:CG2  | 2:O:408:HIS:N     | 2.65                     | 0.59              |
| 1:B:466:LEU:HD22 | 1:B:595:TRP:CZ2   | 2.37                     | 0.59              |
| 1:C:114:CYS:CB   | 9:C:1089:HOH:O    | 2.43                     | 0.59              |
| 2:O:60:TYR:HE2   | 2:O:228:MET:HE3   | 1.68                     | 0.59              |
| 1:C:384:TYR:HD1  | 1:C:384:TYR:H     | 1.51                     | 0.59              |
| 1:D:36:MET:HE1   | 1:D:343:THR:HA    | 1.84                     | 0.59              |
| 2:N:718:LYS:HD2  | 9:N:1200:HOH:O    | 2.03                     | 0.59              |
| 2:M:602:MET:CE   | 2:M:647:ILE:HG21  | 2.33                     | 0.59              |
| 2:O:170:ALA:O    | 2:O:174:LYS:HB2   | 2.02                     | 0.59              |
| 2:P:720:HIS:O    | 2:P:723:LEU:HB2   | 2.03                     | 0.59              |
| 1:B:641:ALA:O    | 1:B:645:ILE:HG13  | 2.02                     | 0.58              |
| 2:O:250:ALA:H    | 2:O:309:ARG:HE    | 1.50                     | 0.58              |
| 2:O:698:LYS:CA   | 2:O:718:LYS:HG2   | 2.29                     | 0.58              |
| 2:P:484:LYS:HA   | 2:P:487:GLU:HG3   | 1.84                     | 0.58              |
| 2:P:565:LYS:HD2  | 2:P:569:ASP:OD1   | 2.03                     | 0.58              |
| 1:D:472:ASN:O    | 1:D:474:LYS:N     | 2.36                     | 0.58              |
| 2:O:516:HIS:HD2  | 2:O:593:THR:OG1   | 1.85                     | 0.58              |
| 1:D:235:ILE:HG23 | 1:D:597:SER:OG    | 2.03                     | 0.58              |
| 2:P:344:GLY:O    | 2:P:346:ARG:NH2   | 2.36                     | 0.58              |
| 2:P:537:LYS:HD3  | 2:P:541:GLU:OE2   | 2.03                     | 0.58              |
| 1:B:102:VAL:CG1  | 5:B:1003[B]:XE:XE | 3.29                     | 0.58              |
| 1:C:280:LEU:HD13 | 1:C:288:SER:HB2   | 1.86                     | 0.58              |
| 2:M:338:MET:SD   | 2:M:341:GLU:HB2   | 2.44                     | 0.58              |
| 2:M:342:MET:HG3  | 2:M:384:LEU:HD22  | 1.86                     | 0.58              |
| 2:M:354:ARG:HD2  | 2:M:389:ASP:OD1   | 2.04                     | 0.58              |
| 2:M:372:ASP:OD1  | 2:M:373:ILE:N     | 2.32                     | 0.58              |
| 2:N:261:VAL:CG1  | 5:N:1006:XE:XE    | 3.30                     | 0.58              |
| 2:O:508:LEU:HD23 | 3:O:900:SF4:S1    | 2.43                     | 0.58              |
| 2:P:144:PHE:O    | 2:P:148:MET:HG3   | 2.02                     | 0.58              |
| 1:C:563:MET:HE1  | 1:C:576:PHE:HD2   | 1.66                     | 0.58              |
| 1:A:278:PHE:HB3  | 1:A:312:LEU:HD23  | 1.84                     | 0.58              |
| 1:A:283:HIS:CD2  | 1:A:317:CYS:HB2   | 2.38                     | 0.58              |
| 2:M:315:LYS:HB2  | 9:M:1182:HOH:O    | 2.02                     | 0.58              |
| 2:O:506:CYS:SG   | 2:O:508:LEU:HB2   | 2.42                     | 0.58              |
| 2:O:525:VAL:HG13 | 2:O:531:VAL:O     | 2.04                     | 0.58              |
| 2:P:602:MET:CE   | 2:P:645:MET:HB3   | 2.34                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:357:SER:OG   | 2:M:360:GLU:HG2  | 2.04                     | 0.58              |
| 2:O:433:ASP:O    | 2:O:437:LYS:HG3  | 2.04                     | 0.58              |
| 2:P:295:VAL:O    | 2:P:295:VAL:HG12 | 2.03                     | 0.58              |
| 2:P:391:TYR:HA   | 2:P:395:MET:HG2  | 1.83                     | 0.58              |
| 2:O:405:ARG:HH22 | 2:O:532:SER:HB3  | 1.67                     | 0.58              |
| 1:C:573:LYS:HE2  | 1:C:671:CYS:O    | 2.04                     | 0.57              |
| 6:D:863:GOL:H12  | 2:P:27:HIS:CE1   | 2.39                     | 0.57              |
| 2:O:156:GLU:HG3  | 2:O:182:MET:HB3  | 1.85                     | 0.57              |
| 1:D:525:LYS:NZ   | 9:D:1094:HOH:O   | 2.33                     | 0.57              |
| 2:M:164:LYS:HD2  | 2:M:298:TYR:CE1  | 2.39                     | 0.57              |
| 1:A:414:SER:O    | 1:A:415:ASN:C    | 2.47                     | 0.57              |
| 2:P:369:ILE:HG22 | 2:P:370:GLY:H    | 1.69                     | 0.57              |
| 1:A:114:CYS:SG   | 1:A:209:HIS:NE2  | 2.77                     | 0.57              |
| 1:C:601:PRO:HD3  | 1:C:652:ARG:CZ   | 2.34                     | 0.57              |
| 2:O:3:ASP:O      | 2:O:6:LYS:HG2    | 2.04                     | 0.57              |
| 2:O:461:ASP:O    | 2:O:462:ARG:HG2  | 2.04                     | 0.57              |
| 2:P:391:TYR:HD2  | 2:P:462:ARG:HH12 | 1.51                     | 0.57              |
| 2:M:716:GLU:HG3  | 2:M:723:LEU:CD1  | 2.35                     | 0.57              |
| 2:N:350:PHE:CD1  | 2:N:350:PHE:C    | 2.83                     | 0.57              |
| 2:N:457:PRO:O    | 2:N:458:ALA:HB3  | 2.03                     | 0.57              |
| 1:B:19:VAL:HG22  | 1:B:474:LYS:HG2  | 1.87                     | 0.57              |
| 2:O:396:GLN:H    | 2:O:399:PHE:HD2  | 1.51                     | 0.57              |
| 2:P:479:GLU:O    | 2:P:481:ALA:N    | 2.37                     | 0.57              |
| 1:D:530:ARG:HG3  | 1:D:530:ARG:HH11 | 1.69                     | 0.57              |
| 2:N:45:ARG:HD2   | 9:N:1216:HOH:O   | 2.03                     | 0.57              |
| 2:O:316:ILE:HG22 | 2:O:454:GLU:OE1  | 2.04                     | 0.57              |
| 1:D:98:VAL:HG21  | 1:D:613:SER:HB3  | 1.87                     | 0.57              |
| 1:D:577:VAL:HG21 | 1:D:645:ILE:HG23 | 1.86                     | 0.56              |
| 2:P:459:ILE:HG22 | 2:P:460:VAL:HG23 | 1.87                     | 0.56              |
| 1:A:602:THR:HG23 | 5:A:1001:XE:XE   | 2.83                     | 0.56              |
| 2:O:389:ASP:HB2  | 2:O:464:GLN:HB3  | 1.87                     | 0.56              |
| 2:P:352:LEU:CD1  | 2:P:353:VAL:O    | 2.54                     | 0.56              |
| 2:P:488:ARG:C    | 2:P:490:ASP:H    | 2.13                     | 0.56              |
| 1:A:114:CYS:SG   | 1:A:209:HIS:CD2  | 2.98                     | 0.56              |
| 1:B:274:ASP:OD1  | 1:B:412:LYS:NZ   | 2.38                     | 0.56              |
| 1:C:126:GLU:HG3  | 1:C:131:LYS:HB2  | 1.87                     | 0.56              |
| 2:M:261:VAL:HG12 | 5:M:1006:XE:XE   | 2.83                     | 0.56              |
| 2:N:21:LEU:HB2   | 2:N:286:LYS:HA   | 1.87                     | 0.56              |
| 2:P:352:LEU:HD11 | 2:P:353:VAL:O    | 2.05                     | 0.56              |
| 2:P:369:ILE:CG2  | 2:P:370:GLY:N    | 2.68                     | 0.56              |
| 2:P:626:MET:HB3  | 2:P:630:THR:HB   | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:313:VAL:HB   | 1:A:331:VAL:HG22 | 1.88                     | 0.56              |
| 1:B:15:GLU:HA    | 6:B:861:GOL:H12  | 1.88                     | 0.56              |
| 1:D:149:ARG:NH2  | 1:D:250:ASP:OD2  | 2.38                     | 0.56              |
| 1:D:357:MET:O    | 1:D:360:ILE:HG12 | 2.05                     | 0.56              |
| 2:M:420:THR:HG22 | 2:M:427:TRP:HB3  | 1.88                     | 0.56              |
| 2:P:478:MET:HE3  | 2:P:482:ARG:HH21 | 1.71                     | 0.56              |
| 2:O:352:LEU:HD23 | 2:O:353:VAL:O    | 2.06                     | 0.56              |
| 2:O:408:HIS:HA   | 2:O:419:HIS:ND1  | 2.21                     | 0.56              |
| 2:O:510:GLN:O    | 2:O:514:PRO:HA   | 2.04                     | 0.56              |
| 2:O:594:SER:HB3  | 2:O:598:PHE:HD2  | 1.70                     | 0.56              |
| 2:P:318:LEU:HD22 | 2:P:320:LEU:HG   | 1.86                     | 0.56              |
| 1:A:213:SER:OG   | 1:B:209:HIS:HD2  | 1.89                     | 0.56              |
| 1:C:217:ASN:HD22 | 1:D:112:ALA:HA   | 1.70                     | 0.56              |
| 1:D:303:LYS:HA   | 1:D:307:ALA:O    | 2.06                     | 0.56              |
| 2:O:359:SER:O    | 2:O:360:GLU:HB2  | 2.06                     | 0.56              |
| 2:O:376:ILE:HG12 | 2:O:382:LEU:HD21 | 1.86                     | 0.56              |
| 2:O:449:VAL:O    | 2:O:449:VAL:HG12 | 2.05                     | 0.56              |
| 2:O:180:GLY:HA2  | 2:O:326:PRO:HG2  | 1.88                     | 0.56              |
| 2:P:347:THR:OG1  | 2:P:383:PRO:HA   | 2.06                     | 0.56              |
| 1:B:190:ILE:HG13 | 1:B:195:LYS:HG3  | 1.86                     | 0.56              |
| 1:B:235:ILE:HD11 | 5:B:1004:XE:XE   | 2.84                     | 0.56              |
| 1:B:334:PHE:O    | 1:B:337:GLN:HG2  | 2.06                     | 0.56              |
| 2:O:66:ARG:HG3   | 2:O:234:PRO:HB3  | 1.86                     | 0.56              |
| 2:P:474:VAL:HG12 | 2:P:475:LYS:H    | 1.71                     | 0.56              |
| 1:D:220:HIS:HD2  | 1:D:221:MET:O    | 1.89                     | 0.56              |
| 2:M:357:SER:OG   | 2:M:360:GLU:CG   | 2.54                     | 0.56              |
| 2:O:478:MET:HG3  | 2:O:482:ARG:HH21 | 1.71                     | 0.56              |
| 2:M:17:GLU:HG2   | 9:M:1179:HOH:O   | 2.05                     | 0.56              |
| 2:O:524:ARG:HH12 | 2:O:645:MET:HE3  | 1.71                     | 0.56              |
| 2:O:564:TRP:HB2  | 2:O:567:VAL:HB   | 1.88                     | 0.56              |
| 2:P:390:ILE:CG1  | 2:P:460:VAL:HG13 | 2.36                     | 0.55              |
| 1:A:2:PRO:N      | 1:A:625:SER:HG   | 2.04                     | 0.55              |
| 1:B:298:MET:CE   | 1:B:301:GLU:OE2  | 2.54                     | 0.55              |
| 2:N:373:ILE:HG12 | 2:N:435:VAL:HG22 | 1.88                     | 0.55              |
| 2:N:486:LYS:HG2  | 9:N:1156:HOH:O   | 2.05                     | 0.55              |
| 2:O:515:ASN:OD1  | 2:O:576:ASN:HB2  | 2.06                     | 0.55              |
| 2:O:522:PRO:HD3  | 2:O:533:TRP:CD1  | 2.41                     | 0.55              |
| 2:P:24:GLU:CD    | 9:P:1085:HOH:O   | 2.50                     | 0.55              |
| 2:P:343:GLY:HA2  | 2:P:347:THR:O    | 2.06                     | 0.55              |
| 2:P:605:LEU:HD22 | 2:P:612:MET:HG2  | 1.88                     | 0.55              |
| 1:C:209:HIS:HD2  | 1:D:213:SER:OG   | 1.89                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:M:108:TYR:O    | 2:M:112:ILE:HG13  | 2.06                     | 0.55              |
| 2:N:341:GLU:HG3  | 2:N:429:ARG:HG2   | 1.89                     | 0.55              |
| 2:P:369:ILE:CG2  | 2:P:370:GLY:H     | 2.20                     | 0.55              |
| 1:A:620:LEU:CD2  | 5:A:1004:XE:XE    | 3.33                     | 0.55              |
| 1:D:504:ALA:O    | 1:D:505:ALA:C     | 2.50                     | 0.55              |
| 2:N:150:ASP:OD1  | 2:N:152:THR:CG2   | 2.55                     | 0.55              |
| 2:O:254:TYR:CZ   | 2:O:258:HIS:CD2   | 2.94                     | 0.55              |
| 2:P:390:ILE:HG13 | 2:P:460:VAL:HG13  | 1.89                     | 0.55              |
| 2:P:479:GLU:C    | 2:P:481:ALA:N     | 2.64                     | 0.55              |
| 2:P:484:LYS:HA   | 2:P:487:GLU:CG    | 2.36                     | 0.55              |
| 1:B:118:ASN:C    | 1:B:118:ASN:HD22  | 2.15                     | 0.55              |
| 1:B:480:SER:HA   | 1:B:638:PRO:HB3   | 1.88                     | 0.55              |
| 2:N:505:SER:HB3  | 2:N:551:ILE:HD11  | 1.87                     | 0.55              |
| 2:O:472:ALA:O    | 2:O:476:GLU:HB2   | 2.07                     | 0.55              |
| 1:B:283:HIS:NE2  | 1:B:587:LYS:NZ    | 2.55                     | 0.55              |
| 2:O:418:TRP:HZ3  | 2:O:429:ARG:NE    | 2.05                     | 0.55              |
| 1:C:281:HIS:HB3  | 1:C:351:VAL:HG12  | 1.89                     | 0.55              |
| 2:M:95:ASN:HD22  | 2:M:95:ASN:C      | 2.15                     | 0.55              |
| 2:P:254:TYR:O    | 2:P:278:THR:HA    | 2.07                     | 0.55              |
| 2:P:373:ILE:HG13 | 2:P:441:PHE:CZ    | 2.42                     | 0.55              |
| 1:A:142:LYS:HD3  | 1:A:253:ASP:HB3   | 1.89                     | 0.55              |
| 1:A:368:HIS:HB2  | 9:A:1141:HOH:O    | 2.06                     | 0.55              |
| 2:M:602:MET:HE3  | 2:M:647:ILE:HG21  | 1.89                     | 0.55              |
| 2:N:95:ASN:ND2   | 2:N:98:ASN:H      | 2.05                     | 0.55              |
| 2:O:670:MET:O    | 2:O:701:ASP:HB3   | 2.07                     | 0.55              |
| 1:A:112:ALA:HA   | 1:B:217:ASN:ND2   | 2.22                     | 0.54              |
| 1:D:470:CYS:N    | 9:D:1085:HOH:O    | 2.39                     | 0.54              |
| 1:B:394:ILE:O    | 1:B:398:LYS:HG3   | 2.07                     | 0.54              |
| 1:C:122:HIS:HD2  | 9:C:1127:HOH:O    | 1.88                     | 0.54              |
| 2:M:615:THR:HG21 | 2:M:674:LEU:HG    | 1.89                     | 0.54              |
| 2:P:21:LEU:HB2   | 2:P:286:LYS:HA    | 1.89                     | 0.54              |
| 2:O:51:HIS:HB3   | 2:O:76:LEU:HD12   | 1.89                     | 0.54              |
| 2:O:525:VAL:HG22 | 2:O:532:SER:HA    | 1.90                     | 0.54              |
| 2:P:338:MET:CE   | 2:P:341:GLU:HB2   | 2.37                     | 0.54              |
| 1:D:620:LEU:HD21 | 5:D:1003[A]:XE:XE | 2.85                     | 0.54              |
| 2:N:568:ASN:HD21 | 2:N:581:GLN:HE21  | 1.55                     | 0.54              |
| 2:N:605:LEU:HD11 | 2:N:612:MET:HB3   | 1.89                     | 0.54              |
| 2:M:426:ASN:C    | 2:M:426:ASN:HD22  | 2.16                     | 0.54              |
| 1:C:587:LYS:N    | 1:D:220:HIS:HE1   | 1.94                     | 0.54              |
| 1:D:208:ILE:HG21 | 9:D:1050:HOH:O    | 2.07                     | 0.54              |
| 1:D:267:ASN:N    | 1:D:330:LEU:O     | 2.41                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:O:593:THR:HB   | 2:O:638:GLY:HA2   | 1.89                     | 0.54              |
| 1:A:72:MET:HG3   | 1:B:105:MET:CE    | 2.37                     | 0.54              |
| 2:O:113:ILE:O    | 2:O:116:LEU:HB2   | 2.07                     | 0.54              |
| 1:D:281:HIS:O    | 1:D:351:VAL:HA    | 2.07                     | 0.54              |
| 2:M:424:ASN:HD22 | 2:M:424:ASN:N     | 2.04                     | 0.54              |
| 2:O:283:PRO:HD2  | 2:O:286:LYS:HB2   | 1.90                     | 0.54              |
| 2:O:402:VAL:C    | 2:O:404:GLU:N     | 2.65                     | 0.54              |
| 2:P:275:PRO:HD2  | 2:P:309:ARG:HD3   | 1.89                     | 0.54              |
| 2:P:319:ASP:O    | 2:P:320:LEU:HB2   | 2.07                     | 0.54              |
| 2:P:479:GLU:C    | 2:P:481:ALA:H     | 2.16                     | 0.54              |
| 2:P:717:GLU:O    | 2:P:717:GLU:HG2   | 2.07                     | 0.54              |
| 1:C:215:LEU:HD13 | 1:C:233:SER:HB3   | 1.89                     | 0.54              |
| 1:D:432:SER:HA   | 1:D:555:ARG:HD3   | 1.90                     | 0.54              |
| 2:M:169:LEU:HD13 | 2:M:193:LEU:HG    | 1.90                     | 0.54              |
| 2:N:583:CYS:HB3  | 2:N:586:THR:HG22  | 1.89                     | 0.54              |
| 2:M:163:ALA:HB2  | 2:M:169:LEU:HG    | 1.90                     | 0.54              |
| 2:N:221:TYR:CD1  | 2:N:221:TYR:C     | 2.86                     | 0.54              |
| 2:O:497:ASP:OD1  | 2:O:523:GLU:HG3   | 2.08                     | 0.54              |
| 2:P:248:ILE:HD12 | 5:P:1008:XE:XE    | 2.86                     | 0.54              |
| 2:P:650:THR:HG22 | 9:P:1070:HOH:O    | 2.08                     | 0.54              |
| 1:A:587:LYS:H    | 1:B:220:HIS:HE1   | 1.56                     | 0.53              |
| 2:N:339:TYR:CD2  | 2:N:435:VAL:HG21  | 2.43                     | 0.53              |
| 2:O:4:PHE:N      | 2:O:238:GLU:OE2   | 2.41                     | 0.53              |
| 2:P:61:TYR:HD2   | 2:P:66:ARG:HD2    | 1.72                     | 0.53              |
| 1:A:32:ALA:O     | 1:A:36:MET:HG2    | 2.08                     | 0.53              |
| 1:B:416:ARG:HG3  | 1:B:416:ARG:NH1   | 2.22                     | 0.53              |
| 1:C:102:VAL:HG11 | 5:C:1003[B]:XE:XE | 2.84                     | 0.53              |
| 2:P:426:ASN:O    | 2:P:427:TRP:HB2   | 2.08                     | 0.53              |
| 1:A:620:LEU:HD21 | 5:A:1003[A]:XE:XE | 2.85                     | 0.53              |
| 1:C:112:ALA:HA   | 1:D:217:ASN:ND2   | 2.24                     | 0.53              |
| 1:C:281:HIS:ND1  | 1:C:282:GLY:N     | 2.57                     | 0.53              |
| 2:N:613:ILE:O    | 2:N:671:PRO:HD3   | 2.07                     | 0.53              |
| 2:O:60:TYR:CE2   | 2:O:228:MET:HE3   | 2.44                     | 0.53              |
| 2:O:488:ARG:C    | 2:O:490:ASP:N     | 2.67                     | 0.53              |
| 2:O:523:GLU:OE2  | 2:O:656:LYS:HE2   | 2.09                     | 0.53              |
| 1:B:510:LEU:N    | 1:B:510:LEU:CD1   | 2.72                     | 0.53              |
| 1:D:98:VAL:HG13  | 1:D:610:VAL:HA    | 1.89                     | 0.53              |
| 2:P:623:PRO:HA   | 2:P:707:THR:HA    | 1.90                     | 0.53              |
| 2:P:670:MET:HE3  | 2:P:675:LYS:HG2   | 1.91                     | 0.53              |
| 2:M:87:ARG:HD2   | 9:M:1010:HOH:O    | 2.07                     | 0.53              |
| 1:A:287:LEU:HD11 | 5:A:1010:XE:XE    | 2.86                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:640:VAL:CG1  | 1:C:644:LYS:HE3  | 2.39                     | 0.53              |
| 1:D:299:GLU:HA   | 1:D:299:GLU:OE1  | 2.09                     | 0.53              |
| 1:D:2:PRO:HA     | 9:D:1040:HOH:O   | 2.09                     | 0.53              |
| 2:M:621:MET:HE1  | 2:M:625:GLY:C    | 2.33                     | 0.53              |
| 2:N:144:PHE:O    | 2:N:148:MET:HG3  | 2.08                     | 0.53              |
| 2:O:345:ASN:C    | 2:O:348:PRO:HD3  | 2.34                     | 0.53              |
| 2:P:341:GLU:OE2  | 2:P:427:TRP:CD1  | 2.61                     | 0.53              |
| 1:C:118:ASN:OD1  | 1:C:209:HIS:HE1  | 1.92                     | 0.53              |
| 2:O:491:ARG:HB2  | 2:O:491:ARG:NH1  | 2.22                     | 0.53              |
| 2:O:686:SER:HB3  | 2:O:692:GLY:O    | 2.09                     | 0.53              |
| 2:P:341:GLU:OE2  | 2:P:427:TRP:HD1  | 1.91                     | 0.53              |
| 2:P:485:TYR:N    | 2:P:485:TYR:CD1  | 2.77                     | 0.53              |
| 1:C:342:CYS:HA   | 1:C:367:TYR:CZ   | 2.44                     | 0.53              |
| 1:C:411:ARG:O    | 1:C:416:ARG:HG2  | 2.08                     | 0.53              |
| 1:A:426:ARG:NH2  | 1:A:539:ILE:HB   | 2.25                     | 0.52              |
| 1:C:615:LEU:HD23 | 1:C:615:LEU:C    | 2.34                     | 0.52              |
| 2:M:424:ASN:H    | 2:M:424:ASN:ND2  | 2.07                     | 0.52              |
| 2:N:527:LEU:HD13 | 2:N:598:PHE:HB3  | 1.91                     | 0.52              |
| 2:P:322:ILE:HG21 | 2:P:434:ALA:HB1  | 1.91                     | 0.52              |
| 2:N:602:MET:HE3  | 2:N:647:ILE:HG21 | 1.91                     | 0.52              |
| 2:O:233:THR:O    | 2:O:240:GLN:NE2  | 2.42                     | 0.52              |
| 2:O:626:MET:HB3  | 2:O:630:THR:HB   | 1.91                     | 0.52              |
| 2:N:417:LEU:O    | 9:N:1164:HOH:O   | 2.19                     | 0.52              |
| 2:O:402:VAL:C    | 2:O:404:GLU:H    | 2.16                     | 0.52              |
| 2:O:434:ALA:O    | 2:O:437:LYS:HB2  | 2.09                     | 0.52              |
| 1:C:633:ILE:HA   | 9:C:1074:HOH:O   | 2.09                     | 0.52              |
| 2:N:156:GLU:HG2  | 5:N:1008:XE:XE   | 2.87                     | 0.52              |
| 2:O:221:TYR:N    | 2:O:224:ARG:HH21 | 2.07                     | 0.52              |
| 2:O:460:VAL:HG13 | 2:O:463:VAL:HG13 | 1.90                     | 0.52              |
| 2:P:395:MET:HE3  | 2:P:396:GLN:O    | 2.09                     | 0.52              |
| 1:B:33:VAL:HG21  | 1:B:477:GLN:HE22 | 1.74                     | 0.52              |
| 2:O:399:PHE:CE1  | 2:O:541:GLU:HG3  | 2.44                     | 0.52              |
| 1:D:28:THR:HG21  | 1:D:33:VAL:HG12  | 1.91                     | 0.52              |
| 2:P:585:TYR:CE1  | 2:P:656:LYS:HD3  | 2.45                     | 0.52              |
| 1:A:96:THR:O     | 1:A:100:ARG:HG3  | 2.10                     | 0.52              |
| 1:C:3:ARG:HG3    | 1:C:3:ARG:HH11   | 1.75                     | 0.52              |
| 1:D:118:ASN:C    | 1:D:118:ASN:HD22 | 2.17                     | 0.52              |
| 2:P:525:VAL:HB   | 9:P:1069:HOH:O   | 2.09                     | 0.52              |
| 1:A:506:GLY:CA   | 1:A:511:LEU:HD12 | 2.39                     | 0.52              |
| 2:O:136:ILE:HG21 | 2:O:221:TYR:CE2  | 2.45                     | 0.52              |
| 2:O:549:GLN:HB3  | 2:O:550:PRO:CD   | 2.40                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:554:GLU:HG3  | 2:O:566:SER:HB3  | 1.90                     | 0.52              |
| 2:O:657:PHE:HE2  | 2:O:667:ILE:HD11 | 1.75                     | 0.52              |
| 1:B:577:VAL:HG12 | 1:B:601:PRO:HG2  | 1.92                     | 0.52              |
| 1:C:68:CYS:HB2   | 1:C:97:ILE:HG23  | 1.92                     | 0.52              |
| 1:C:396:SER:HB3  | 5:C:1010:XE:XE   | 2.88                     | 0.52              |
| 1:C:500:CYS:HA   | 1:C:503:GLN:HG3  | 1.91                     | 0.52              |
| 2:N:95:ASN:C     | 2:N:95:ASN:HD22  | 2.17                     | 0.52              |
| 2:O:672:LYS:C    | 2:O:674:LEU:H    | 2.16                     | 0.52              |
| 2:P:364:GLY:N    | 2:P:463:VAL:O    | 2.42                     | 0.52              |
| 1:A:177:LEU:HB2  | 1:A:180:GLU:CD   | 2.35                     | 0.52              |
| 1:C:563:MET:HE2  | 1:C:576:PHE:CD2  | 2.44                     | 0.52              |
| 2:O:356:VAL:HG11 | 2:O:360:GLU:OE2  | 2.10                     | 0.52              |
| 2:P:142:ARG:HG2  | 2:P:142:ARG:HH11 | 1.75                     | 0.52              |
| 2:P:333:ILE:HD12 | 2:P:418:TRP:HB2  | 1.92                     | 0.52              |
| 2:P:681:GLU:CG   | 2:P:684:ARG:HH21 | 2.23                     | 0.52              |
| 1:B:572:PRO:HG3  | 1:B:629:GLY:HA3  | 1.92                     | 0.51              |
| 1:C:220:HIS:O    | 1:C:223:MET:HB2  | 2.11                     | 0.51              |
| 1:D:283:HIS:CD2  | 1:D:317:CYS:HB2  | 2.45                     | 0.51              |
| 2:O:183:LEU:HB2  | 2:O:206:ALA:HA   | 1.93                     | 0.51              |
| 2:O:351:GLU:HG3  | 2:O:423:ARG:HA   | 1.92                     | 0.51              |
| 2:O:508:LEU:CB   | 3:O:900:SF4:S1   | 2.95                     | 0.51              |
| 2:O:590:ASN:N    | 2:O:591:PRO:HD3  | 2.26                     | 0.51              |
| 2:P:412:ASN:ND2  | 2:P:419:HIS:HB3  | 2.25                     | 0.51              |
| 1:C:9:HIS:CD2    | 1:C:644:LYS:HG2  | 2.45                     | 0.51              |
| 1:D:332:THR:OG1  | 1:D:336:SER:OG   | 2.26                     | 0.51              |
| 2:M:246:ARG:HE   | 2:M:247:ARG:NH1  | 2.08                     | 0.51              |
| 2:N:408:HIS:HD2  | 2:N:419:HIS:ND1  | 2.08                     | 0.51              |
| 2:O:382:LEU:HD23 | 2:O:469:THR:HG21 | 1.91                     | 0.51              |
| 2:P:568:ASN:HD21 | 2:P:581:GLN:CG   | 2.22                     | 0.51              |
| 1:C:114:CYS:HB2  | 1:C:208:ILE:HG21 | 1.92                     | 0.51              |
| 2:M:95:ASN:HD21  | 2:M:98:ASN:H     | 1.57                     | 0.51              |
| 1:D:191:ASN:ND2  | 9:D:1034:HOH:O   | 2.42                     | 0.51              |
| 2:O:344:GLY:O    | 2:O:346:ARG:NH1  | 2.44                     | 0.51              |
| 2:P:229:PHE:CD1  | 5:P:1009:XE:XE   | 3.41                     | 0.51              |
| 1:B:256:PHE:CD1  | 1:B:289:GLU:HG3  | 2.46                     | 0.51              |
| 1:D:292:VAL:HG11 | 1:D:326:GLN:HG3  | 1.93                     | 0.51              |
| 1:C:611:GLU:HB2  | 9:C:1122:HOH:O   | 2.10                     | 0.51              |
| 1:D:105:MET:HE2  | 1:D:609:PRO:HG3  | 1.92                     | 0.51              |
| 2:O:152:THR:O    | 2:O:154:PRO:HD3  | 2.11                     | 0.51              |
| 2:O:224:ARG:O    | 2:O:228:MET:HB2  | 2.10                     | 0.51              |
| 2:O:524:ARG:HB2  | 2:O:651:TYR:CE1  | 2.46                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:620:LEU:HD23 | 5:A:1004:XE:XE   | 2.88                     | 0.51              |
| 2:O:254:TYR:CE2  | 2:O:258:HIS:CD2  | 2.98                     | 0.51              |
| 2:O:430:VAL:HG11 | 2:O:439:PHE:CE2  | 2.45                     | 0.51              |
| 2:P:343:GLY:O    | 2:P:346:ARG:NH1  | 2.43                     | 0.51              |
| 1:D:68:CYS:HB2   | 1:D:97:ILE:HG23  | 1.93                     | 0.51              |
| 2:N:335:LYS:HD3  | 2:N:429:ARG:HH12 | 1.76                     | 0.51              |
| 2:O:277:ILE:N    | 2:O:277:ILE:HD12 | 2.25                     | 0.51              |
| 2:P:288:ILE:O    | 2:P:289:PRO:C    | 2.54                     | 0.51              |
| 2:O:612:MET:SD   | 2:O:622:THR:HB   | 2.51                     | 0.51              |
| 2:P:385:GLY:O    | 2:P:467:ILE:HA   | 2.11                     | 0.51              |
| 2:P:602:MET:HE2  | 2:P:647:ILE:HG21 | 1.93                     | 0.51              |
| 1:A:592:GLY:HA2  | 5:A:1001:XE:XE   | 2.89                     | 0.51              |
| 1:B:394:ILE:HG23 | 1:B:395:GLU:H    | 1.76                     | 0.51              |
| 2:O:26:TYR:CE1   | 2:O:30:ILE:HD11  | 2.46                     | 0.51              |
| 2:O:122:LYS:HB2  | 2:O:125:GLU:HG3  | 1.93                     | 0.51              |
| 2:P:340:VAL:HG13 | 2:P:341:GLU:N    | 2.26                     | 0.51              |
| 1:A:220:HIS:HD2  | 1:A:221:MET:O    | 1.94                     | 0.50              |
| 1:B:298:MET:HE1  | 1:B:301:GLU:OE2  | 2.10                     | 0.50              |
| 2:M:62:LEU:HD13  | 2:M:115:ALA:HB2  | 1.93                     | 0.50              |
| 2:O:527:LEU:HA   | 2:O:648:GLY:N    | 2.26                     | 0.50              |
| 2:P:403:LEU:N    | 2:P:403:LEU:HD23 | 2.26                     | 0.50              |
| 2:P:564:TRP:HB2  | 2:P:567:VAL:HB   | 1.93                     | 0.50              |
| 2:P:626:MET:SD   | 2:P:634:MET:HE3  | 2.52                     | 0.50              |
| 1:A:72:MET:HG3   | 1:B:105:MET:HE1  | 1.93                     | 0.50              |
| 1:D:266:ALA:HA   | 1:D:330:LEU:O    | 2.12                     | 0.50              |
| 2:M:373:ILE:HG22 | 2:M:440:ARG:HD3  | 1.93                     | 0.50              |
| 2:O:259:ASP:OD2  | 2:O:262:LYS:HD2  | 2.11                     | 0.50              |
| 2:N:693:GLU:CD   | 2:N:693:GLU:H    | 2.19                     | 0.50              |
| 2:O:391:TYR:HD2  | 2:O:462:ARG:HB2  | 1.77                     | 0.50              |
| 1:A:217:ASN:ND2  | 1:B:112:ALA:HA   | 2.26                     | 0.50              |
| 1:A:305:ALA:HB1  | 1:A:409:LYS:HD2  | 1.93                     | 0.50              |
| 1:B:620:LEU:CD2  | 5:B:1004:XE:XE   | 3.38                     | 0.50              |
| 1:D:241:ASP:OD1  | 1:D:241:ASP:C    | 2.54                     | 0.50              |
| 2:M:586:THR:HG1  | 2:M:661:ASP:CG   | 2.17                     | 0.50              |
| 2:M:704:ILE:C    | 2:M:704:ILE:HD12 | 2.36                     | 0.50              |
| 2:O:269:ALA:HB1  | 2:O:274:PHE:HB2  | 1.93                     | 0.50              |
| 2:P:338:MET:HE3  | 2:P:341:GLU:HB2  | 1.91                     | 0.50              |
| 2:P:358:GLU:HA   | 2:P:361:ILE:HG22 | 1.92                     | 0.50              |
| 1:D:307:ALA:HB2  | 1:D:408:PHE:CE2  | 2.46                     | 0.50              |
| 1:B:372:ILE:CD1  | 1:B:403:MET:HE3  | 2.40                     | 0.50              |
| 1:D:127:MET:SD   | 1:D:127:MET:C    | 2.95                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:275:GLN:HG2  | 1:D:309:GLY:O    | 2.11                     | 0.50              |
| 1:D:615:LEU:H    | 6:D:863:GOL:C1   | 2.25                     | 0.50              |
| 2:M:373:ILE:HG21 | 2:M:439:PHE:O    | 2.11                     | 0.50              |
| 2:N:679:HIS:HD2  | 2:N:680:ASP:OD1  | 1.94                     | 0.50              |
| 1:B:620:LEU:HD22 | 5:B:1004:XE:XE   | 2.90                     | 0.50              |
| 1:D:146:VAL:O    | 1:D:150:VAL:HG22 | 2.11                     | 0.50              |
| 1:D:267:ASN:O    | 1:D:270:VAL:HG22 | 2.11                     | 0.50              |
| 1:D:416:ARG:HB2  | 1:D:418:VAL:CG2  | 2.42                     | 0.50              |
| 2:O:166:SER:HB3  | 2:O:192:GLN:HB3  | 1.93                     | 0.50              |
| 2:O:362:THR:HB   | 2:O:365:LYS:HB2  | 1.94                     | 0.50              |
| 2:O:392:GLY:HA2  | 2:O:461:ASP:HB2  | 1.93                     | 0.50              |
| 2:O:725:MET:O    | 2:O:726:ASP:HB3  | 2.11                     | 0.50              |
| 1:B:32:ALA:O     | 1:B:36:MET:HG2   | 2.11                     | 0.50              |
| 1:D:41:LYS:O     | 1:D:41:LYS:HG2   | 2.12                     | 0.50              |
| 1:B:341:ILE:HA   | 1:B:346:ILE:HG12 | 1.93                     | 0.50              |
| 1:C:202:ASN:HA   | 9:C:1120:HOH:O   | 2.11                     | 0.50              |
| 1:D:105:MET:HE1  | 1:D:609:PRO:HD3  | 1.88                     | 0.50              |
| 2:N:272:THR:HG22 | 2:N:272:THR:O    | 2.11                     | 0.50              |
| 1:B:549:SER:HB2  | 9:B:1019:HOH:O   | 2.12                     | 0.49              |
| 2:O:95:ASN:C     | 2:O:95:ASN:HD22  | 2.20                     | 0.49              |
| 2:O:497:ASP:HB2  | 2:O:656:LYS:NZ   | 2.28                     | 0.49              |
| 2:O:597:CYS:SG   | 3:O:900:SF4:S3   | 3.10                     | 0.49              |
| 2:P:353:VAL:HG13 | 2:P:388:VAL:HB   | 1.93                     | 0.49              |
| 1:C:584:MET:O    | 1:D:71:CYS:HB2   | 2.11                     | 0.49              |
| 2:N:602:MET:CE   | 2:N:647:ILE:HG21 | 2.42                     | 0.49              |
| 2:O:144:PHE:O    | 2:O:148:MET:CG   | 2.49                     | 0.49              |
| 2:O:163:ALA:HB2  | 2:O:255:LEU:HD13 | 1.92                     | 0.49              |
| 2:O:373:ILE:C    | 2:O:375:GLN:H    | 2.20                     | 0.49              |
| 2:O:504:TYR:OH   | 2:O:537:LYS:HG2  | 2.11                     | 0.49              |
| 2:O:508:LEU:C    | 2:O:510:GLN:H    | 2.19                     | 0.49              |
| 2:O:529:GLY:HA3  | 2:O:599:GLU:OE2  | 2.12                     | 0.49              |
| 2:O:669:TRP:HD1  | 2:O:711:ILE:HG21 | 1.78                     | 0.49              |
| 2:P:275:PRO:CD   | 2:P:309:ARG:HD3  | 2.42                     | 0.49              |
| 2:P:391:TYR:CD2  | 2:P:462:ARG:NH1  | 2.78                     | 0.49              |
| 2:P:403:LEU:HD22 | 2:P:456:PHE:CZ   | 2.48                     | 0.49              |
| 2:P:525:VAL:HG11 | 2:P:650:THR:HG22 | 1.95                     | 0.49              |
| 1:C:579:SER:HA   | 1:C:603:HIS:O    | 2.12                     | 0.49              |
| 2:O:136:ILE:HG21 | 2:O:221:TYR:HE2  | 1.77                     | 0.49              |
| 2:O:508:LEU:N    | 3:O:900:SF4:S2   | 2.84                     | 0.49              |
| 1:C:220:HIS:HE1  | 1:D:587:LYS:H    | 1.61                     | 0.49              |
| 1:D:317:CYS:O    | 1:D:321:GLU:HG2  | 2.11                     | 0.49              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:M:184:PHE:C    | 2:M:185:ILE:HG13   | 2.36                     | 0.49              |
| 2:M:373:ILE:CG2  | 2:M:440:ARG:HA     | 2.43                     | 0.49              |
| 2:N:621:MET:HE1  | 9:N:1020:HOH:O     | 2.12                     | 0.49              |
| 2:P:674:LEU:O    | 2:P:678:LEU:HD12   | 2.12                     | 0.49              |
| 1:A:281:HIS:HB3  | 1:A:351:VAL:HG12   | 1.94                     | 0.49              |
| 1:B:386:ILE:HD11 | 1:B:403:MET:HE1    | 1.95                     | 0.49              |
| 1:C:18:ARG:NE    | 1:C:636:MET:HE3    | 2.28                     | 0.49              |
| 1:D:282:GLY:HA3  | 1:D:352:ASP:OD1    | 2.13                     | 0.49              |
| 1:D:333:SER:HA   | 1:D:503:GLN:NE2    | 2.28                     | 0.49              |
| 2:N:365:LYS:HB3  | 2:N:464:GLN:HG3    | 1.95                     | 0.49              |
| 2:O:184:PHE:HB3  | 2:O:209:LEU:HD11   | 1.95                     | 0.49              |
| 2:O:457:PRO:O    | 2:O:458:ALA:CB     | 2.60                     | 0.49              |
| 2:P:472:ALA:O    | 2:P:476:GLU:HB2    | 2.13                     | 0.49              |
| 1:D:285:PRO:C    | 1:D:287:LEU:N      | 2.69                     | 0.49              |
| 2:O:150:ASP:OD2  | 2:O:152:THR:HG23   | 2.13                     | 0.49              |
| 2:O:579:LEU:HD22 | 2:O:593:THR:CG2    | 2.42                     | 0.49              |
| 2:P:373:ILE:HD13 | 2:P:435:VAL:HG22   | 1.94                     | 0.49              |
| 1:A:443:GLN:HB2  | 1:A:451:VAL:HG21   | 1.94                     | 0.49              |
| 2:O:649:ARG:HA   | 2:O:652:ILE:HD12   | 1.94                     | 0.49              |
| 2:P:261:VAL:HG12 | 5:P:1006:XE:XE     | 2.91                     | 0.49              |
| 1:A:571:THR:OG1  | 1:A:572:PRO:HD3    | 2.13                     | 0.49              |
| 2:N:558:ASP:C    | 2:N:558:ASP:OD1    | 2.56                     | 0.49              |
| 1:C:52:PHE:CZ    | 1:C:474:LYS:HA     | 2.48                     | 0.48              |
| 2:O:138:ASP:HB2  | 2:O:139:PRO:HD3    | 1.95                     | 0.48              |
| 2:O:250:ALA:N    | 2:O:309:ARG:HE     | 2.10                     | 0.48              |
| 2:O:416:GLY:O    | 2:O:430:VAL:HA     | 2.13                     | 0.48              |
| 1:C:563:MET:CE   | 1:C:576:PHE:CD2    | 2.88                     | 0.48              |
| 1:D:164:GLN:O    | 1:D:168[A]:GLU:HG3 | 2.12                     | 0.48              |
| 2:O:316:ILE:CG2  | 2:O:454:GLU:OE1    | 2.61                     | 0.48              |
| 2:O:649:ARG:C    | 2:O:651:TYR:H      | 2.20                     | 0.48              |
| 2:P:354:ARG:HG2  | 2:P:484:LYS:NZ     | 2.28                     | 0.48              |
| 2:P:605:LEU:HD11 | 2:P:624:SER:HA     | 1.95                     | 0.48              |
| 2:O:19:VAL:O     | 2:O:22:PHE:HB2     | 2.13                     | 0.48              |
| 2:O:66:ARG:HG3   | 2:O:66:ARG:O       | 2.12                     | 0.48              |
| 2:O:602:MET:HE3  | 2:O:645:MET:HB3    | 1.94                     | 0.48              |
| 2:P:170:ALA:O    | 2:P:174:LYS:HB2    | 2.13                     | 0.48              |
| 2:P:667:ILE:O    | 2:P:699:ILE:HG12   | 2.13                     | 0.48              |
| 2:P:681:GLU:HG3  | 2:P:684:ARG:NH2    | 2.28                     | 0.48              |
| 1:B:587:LYS:HE3  | 4:B:800:XCC:S4     | 2.53                     | 0.48              |
| 1:C:596:VAL:HG21 | 1:C:632:PHE:CE2    | 2.48                     | 0.48              |
| 2:O:261:VAL:HG12 | 5:O:1006:XE:XE     | 2.91                     | 0.48              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:P:343:GLY:HA3    | 2:P:349:ALA:CB   | 2.39                     | 0.48              |
| 1:C:540:GLY:HA2    | 9:C:1136:HOH:O   | 2.13                     | 0.48              |
| 2:N:182:MET:HB2    | 2:N:182:MET:HE3  | 1.67                     | 0.48              |
| 2:O:449:VAL:O      | 2:O:449:VAL:CG1  | 2.62                     | 0.48              |
| 2:O:657:PHE:CE2    | 2:O:667:ILE:HD11 | 2.48                     | 0.48              |
| 2:P:585:TYR:CZ     | 2:P:656:LYS:HD3  | 2.49                     | 0.48              |
| 2:M:716:GLU:HG3    | 2:M:723:LEU:HD12 | 1.95                     | 0.48              |
| 2:O:7:ILE:HD12     | 2:O:245:ARG:HD2  | 1.96                     | 0.48              |
| 2:O:270:ILE:O      | 2:O:271:PHE:C    | 2.55                     | 0.48              |
| 2:P:339:TYR:CD1    | 2:P:339:TYR:C    | 2.91                     | 0.48              |
| 2:P:350:PHE:CD1    | 2:P:351:GLU:N    | 2.82                     | 0.48              |
| 1:A:370:ARG:HG2    | 1:A:370:ARG:HH11 | 1.79                     | 0.48              |
| 1:B:415:ASN:CG     | 1:B:415:ASN:O    | 2.57                     | 0.48              |
| 2:O:215:ILE:HG21   | 5:O:1006:XE:XE   | 2.92                     | 0.48              |
| 2:P:95:ASN:C       | 2:P:95:ASN:ND2   | 2.56                     | 0.48              |
| 1:A:272:ASP:C      | 1:A:272:ASP:OD1  | 2.56                     | 0.48              |
| 1:A:506:GLY:HA2    | 1:A:511:LEU:HD12 | 1.96                     | 0.48              |
| 1:C:112:ALA:HA     | 1:D:217:ASN:HD22 | 1.79                     | 0.48              |
| 1:C:384:TYR:CD1    | 1:C:384:TYR:N    | 2.80                     | 0.48              |
| 1:D:147:CYS:HB3    | 1:D:152:ILE:HB   | 1.95                     | 0.48              |
| 1:D:275:GLN:HG2    | 1:D:309:GLY:C    | 2.39                     | 0.48              |
| 2:O:229:PHE:CD1    | 5:O:1009:XE:XE   | 3.45                     | 0.48              |
| 2:O:289:PRO:C      | 2:O:291:TRP:H    | 2.21                     | 0.48              |
| 2:P:221:TYR:CD1    | 2:P:221:TYR:C    | 2.91                     | 0.48              |
| 2:P:341:GLU:HG3    | 2:P:429:ARG:HB3  | 1.95                     | 0.48              |
| 1:A:384:TYR:CD2    | 2:N:84:ASN:HB3   | 2.49                     | 0.48              |
| 1:B:443:GLN:HB2    | 1:B:451:VAL:HG21 | 1.96                     | 0.48              |
| 1:C:569:VAL:CG1    | 1:C:573:LYS:HD3  | 2.43                     | 0.48              |
| 2:N:340:VAL:HG22   | 2:N:341:GLU:N    | 2.29                     | 0.48              |
| 2:O:556:GLU:HG3    | 2:O:564:TRP:NE1  | 2.29                     | 0.48              |
| 2:P:576:ASN:O      | 2:P:577:ARG:HB2  | 2.14                     | 0.48              |
| 1:C:563:MET:HE3    | 1:C:574:VAL:HG11 | 1.96                     | 0.48              |
| 2:O:408:HIS:HA     | 2:O:419:HIS:HD1  | 1.77                     | 0.48              |
| 2:O:503:PHE:O      | 2:O:551:ILE:N    | 2.36                     | 0.48              |
| 2:O:685:ARG:HA     | 2:O:688:GLU:HB2  | 1.95                     | 0.48              |
| 2:P:117[A]:ARG:NH2 | 9:P:1051:HOH:O   | 2.47                     | 0.48              |
| 2:P:701:ASP:O      | 2:P:702:GLU:C    | 2.57                     | 0.48              |
| 1:B:394:ILE:HG23   | 1:B:395:GLU:N    | 2.29                     | 0.47              |
| 1:C:3:ARG:HG3      | 1:C:3:ARG:NH1    | 2.29                     | 0.47              |
| 1:C:384:TYR:HD1    | 1:C:384:TYR:N    | 2.11                     | 0.47              |
| 2:N:568:ASN:ND2    | 2:N:581:GLN:HE21 | 2.11                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:485:TYR:HA   | 2:O:489:ASP:HB2  | 1.95                     | 0.47              |
| 2:P:665:ALA:O    | 2:P:720:HIS:HE1  | 1.97                     | 0.47              |
| 1:A:576:PHE:CD1  | 1:A:576:PHE:C    | 2.93                     | 0.47              |
| 1:B:241:ASP:OD1  | 1:B:245:GLU:OE2  | 2.31                     | 0.47              |
| 1:B:426:ARG:NH2  | 9:B:1216:HOH:O   | 2.46                     | 0.47              |
| 1:D:46:ILE:HD12  | 6:D:860:GOL:H31  | 1.95                     | 0.47              |
| 2:O:335:LYS:HD2  | 2:O:336:GLY:N    | 2.28                     | 0.47              |
| 1:A:267:ASN:O    | 1:A:270:VAL:HG22 | 2.13                     | 0.47              |
| 1:A:559:LEU:HG   | 1:A:563:MET:HE2  | 1.97                     | 0.47              |
| 1:A:601:PRO:HD3  | 1:A:652:ARG:CZ   | 2.45                     | 0.47              |
| 1:A:607:MET:HE3  | 1:A:611:GLU:CD   | 2.39                     | 0.47              |
| 2:N:244:GLN:HG3  | 2:N:272:THR:CG2  | 2.45                     | 0.47              |
| 1:A:658:VAL:O    | 1:A:662:VAL:HG23 | 2.15                     | 0.47              |
| 1:C:420:ILE:O    | 1:C:421:PRO:C    | 2.56                     | 0.47              |
| 2:N:187:ASP:HA   | 2:N:211:ASN:ND2  | 2.24                     | 0.47              |
| 2:N:527:LEU:HD12 | 2:N:527:LEU:C    | 2.40                     | 0.47              |
| 2:P:354:ARG:HD2  | 2:P:355:THR:H    | 1.79                     | 0.47              |
| 2:P:491:ARG:O    | 2:P:495:LEU:HD12 | 2.15                     | 0.47              |
| 2:P:527:LEU:HA   | 2:P:648:GLY:N    | 2.30                     | 0.47              |
| 1:D:114:CYS:CA   | 9:D:1050:HOH:O   | 2.62                     | 0.47              |
| 1:D:466:LEU:HD22 | 1:D:595:TRP:CZ2  | 2.49                     | 0.47              |
| 2:O:295:VAL:CG1  | 2:O:301:ILE:HG12 | 2.45                     | 0.47              |
| 2:O:376:ILE:HG21 | 2:O:382:LEU:HD11 | 1.97                     | 0.47              |
| 2:O:418:TRP:CZ3  | 2:O:429:ARG:NE   | 2.82                     | 0.47              |
| 1:B:317:CYS:O    | 1:B:321:GLU:HG2  | 2.15                     | 0.47              |
| 1:B:654:TRP:HE1  | 2:N:195:GLU:CD   | 2.23                     | 0.47              |
| 1:C:154:VAL:HG13 | 1:C:162:LEU:HD11 | 1.97                     | 0.47              |
| 1:C:545:PHE:N    | 1:C:545:PHE:CD1  | 2.83                     | 0.47              |
| 1:D:278:PHE:HB3  | 1:D:312:LEU:HD23 | 1.96                     | 0.47              |
| 2:O:276:VAL:N    | 2:O:291:TRP:O    | 2.46                     | 0.47              |
| 2:P:150:ASP:OD1  | 2:P:152:THR:CG2  | 2.62                     | 0.47              |
| 2:P:400:GLU:C    | 2:P:402:VAL:H    | 2.21                     | 0.47              |
| 2:P:412:ASN:OD1  | 2:P:418:TRP:HA   | 2.13                     | 0.47              |
| 2:P:589:GLU:O    | 2:P:590:ASN:C    | 2.58                     | 0.47              |
| 1:C:43:ASP:O     | 1:C:44:LYS:HB2   | 2.15                     | 0.47              |
| 1:C:107:LEU:HD21 | 1:C:215:LEU:HB3  | 1.96                     | 0.47              |
| 1:C:126:GLU:HG2  | 1:C:132:ALA:HB2  | 1.97                     | 0.47              |
| 1:C:318:THR:O    | 1:C:322:VAL:HG22 | 2.15                     | 0.47              |
| 1:D:52:PHE:CZ    | 1:D:474:LYS:HA   | 2.50                     | 0.47              |
| 1:D:82:ASP:OD1   | 1:D:83:GLY:N     | 2.44                     | 0.47              |
| 2:M:340:VAL:HG22 | 2:M:341:GLU:N    | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:162:ARG:HB2  | 2:N:188:GLU:HB2  | 1.96                     | 0.47              |
| 2:O:66:ARG:CZ    | 2:O:234:PRO:HG2  | 2.45                     | 0.47              |
| 2:O:107:TRP:NE1  | 2:O:268:GLY:HA3  | 2.29                     | 0.47              |
| 2:O:118:TYR:CD2  | 2:O:121:TYR:HB2  | 2.50                     | 0.47              |
| 2:O:162:ARG:HG3  | 2:O:188:GLU:HB2  | 1.97                     | 0.47              |
| 2:O:334:ARG:O    | 2:O:335:LYS:C    | 2.57                     | 0.47              |
| 1:A:191:ASN:OD1  | 1:A:194:ARG:HG2  | 2.14                     | 0.47              |
| 1:D:447:ASN:ND2  | 1:D:450:ARG:HB2  | 2.30                     | 0.47              |
| 2:M:315:LYS:HG3  | 9:M:1153:HOH:O   | 2.14                     | 0.47              |
| 2:O:563:ILE:HG12 | 2:O:583:CYS:SG   | 2.55                     | 0.47              |
| 2:P:339:TYR:HB2  | 2:P:432:LYS:HA   | 1.96                     | 0.47              |
| 1:C:292:VAL:HA   | 1:C:312:LEU:HD11 | 1.96                     | 0.47              |
| 2:M:150:ASP:OD1  | 2:M:152:THR:CG2  | 2.62                     | 0.47              |
| 2:M:341:GLU:HG3  | 2:M:429:ARG:HG2  | 1.97                     | 0.47              |
| 2:M:675:LYS:NZ   | 2:M:699:ILE:O    | 2.40                     | 0.47              |
| 2:P:354:ARG:HH21 | 2:P:356:VAL:HG11 | 1.73                     | 0.47              |
| 1:A:287:LEU:HD13 | 1:A:388:TYR:CE1  | 2.50                     | 0.47              |
| 1:D:182:GLU:OE2  | 1:D:199:ARG:HD3  | 2.15                     | 0.47              |
| 1:D:373:THR:CG2  | 1:D:380:ILE:HD12 | 2.45                     | 0.47              |
| 2:M:129:PRO:O    | 2:M:132:TRP:HB2  | 2.15                     | 0.47              |
| 2:O:71:GLU:HG3   | 2:O:82:ILE:HD11  | 1.96                     | 0.47              |
| 2:O:86:LYS:HA    | 2:O:86:LYS:HD3   | 1.62                     | 0.47              |
| 2:P:490:ASP:O    | 2:P:492:MET:N    | 2.48                     | 0.47              |
| 1:C:223:MET:SD   | 1:D:353:VAL:HB   | 2.54                     | 0.46              |
| 2:M:206:ALA:O    | 2:M:208:PRO:HD3  | 2.15                     | 0.46              |
| 2:O:124:ASP:OD1  | 2:O:124:ASP:N    | 2.40                     | 0.46              |
| 1:C:279:VAL:HG22 | 1:C:313:VAL:HG23 | 1.96                     | 0.46              |
| 1:D:30:ASP:HA    | 1:D:508:LEU:HD21 | 1.97                     | 0.46              |
| 2:N:381:LYS:HE2  | 2:N:381:LYS:HB2  | 1.43                     | 0.46              |
| 2:N:681:GLU:HB3  | 2:N:684:ARG:NH2  | 2.29                     | 0.46              |
| 2:O:181:PHE:CE1  | 2:O:251:PHE:HE2  | 2.33                     | 0.46              |
| 2:O:220:ASN:C    | 2:O:224:ARG:HH21 | 2.24                     | 0.46              |
| 2:O:427:TRP:O    | 2:O:428:LEU:HB2  | 2.13                     | 0.46              |
| 2:O:488:ARG:HB3  | 2:O:488:ARG:NH1  | 2.30                     | 0.46              |
| 2:P:343:GLY:CA   | 2:P:349:ALA:HB3  | 2.40                     | 0.46              |
| 1:B:607:MET:HG3  | 1:B:608:PRO:O    | 2.15                     | 0.46              |
| 1:D:25:ARG:NH2   | 1:D:41:LYS:HB2   | 2.30                     | 0.46              |
| 2:M:560:ILE:O    | 2:M:660:ALA:HB2  | 2.15                     | 0.46              |
| 2:M:704:ILE:HD12 | 2:M:704:ILE:O    | 2.15                     | 0.46              |
| 1:B:20:MET:HG3   | 9:B:1052:HOH:O   | 2.14                     | 0.46              |
| 1:D:129:GLU:OE2  | 1:D:164:GLN:NE2  | 2.49                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:D:477:GLN:O      | 1:D:478:ASP:HB2     | 2.15                     | 0.46              |
| 2:M:383:PRO:HG3    | 2:M:471:GLU:HG2     | 1.98                     | 0.46              |
| 2:M:408:HIS:CD2    | 2:M:419:HIS:ND1     | 2.78                     | 0.46              |
| 2:N:211:ASN:ND2    | 9:N:1016:HOH:O      | 2.39                     | 0.46              |
| 2:N:657:PHE:O      | 2:N:663:GLY:HA2     | 2.15                     | 0.46              |
| 2:O:169:LEU:HD13   | 2:O:193:LEU:HD21    | 1.97                     | 0.46              |
| 2:P:488:ARG:HG2    | 2:P:491:ARG:NH2     | 2.30                     | 0.46              |
| 1:D:107:LEU:HD21   | 1:D:215:LEU:HB3     | 1.98                     | 0.46              |
| 1:D:555:ARG:HG2    | 9:D:1045:HOH:O      | 2.15                     | 0.46              |
| 2:N:283:PRO:HG2    | 2:N:286:LYS:HG3     | 1.96                     | 0.46              |
| 2:O:193:LEU:HD22   | 2:O:198:VAL:HG21    | 1.98                     | 0.46              |
| 2:P:571:LEU:HD12   | 2:P:575:SER:HB3     | 1.97                     | 0.46              |
| 1:B:87:ARG:HD3     | 1:B:91:GLY:O        | 2.16                     | 0.46              |
| 1:D:145:GLU:OE1    | 1:D:145:GLU:HA      | 2.16                     | 0.46              |
| 2:M:611:ILE:HD11   | 2:M:667:ILE:HG12    | 1.98                     | 0.46              |
| 2:N:147:LYS:HB3    | 2:N:153:ILE:HD12    | 1.96                     | 0.46              |
| 2:N:540:TYR:CE1    | 2:N:544:HIS:HA      | 2.51                     | 0.46              |
| 2:O:333:ILE:HG13   | 2:O:418:TRP:HB2     | 1.98                     | 0.46              |
| 2:O:603:ALA:HB3    | 2:O:612:MET:HG3     | 1.97                     | 0.46              |
| 2:P:553:LYS:HG2    | 2:P:564:TRP:NE1     | 2.30                     | 0.46              |
| 1:A:217:ASN:HD22   | 1:B:112:ALA:HA      | 1.81                     | 0.46              |
| 1:B:7:LEU:HD11     | 2:N:164:LYS:HB2     | 1.97                     | 0.46              |
| 1:B:661[A]:GLU:HG3 | 1:B:665[A]:ARG:HH21 | 1.80                     | 0.46              |
| 2:N:681:GLU:HB3    | 2:N:684:ARG:HH21    | 1.80                     | 0.46              |
| 2:O:354:ARG:HE     | 2:O:356:VAL:HG22    | 1.81                     | 0.46              |
| 2:P:316:ILE:O      | 2:P:316:ILE:CG2     | 2.61                     | 0.46              |
| 2:P:602:MET:HE2    | 2:P:647:ILE:CG2     | 2.45                     | 0.46              |
| 1:D:416:ARG:C      | 1:D:418:VAL:H       | 2.24                     | 0.46              |
| 2:O:79:LEU:O       | 2:O:80:PRO:C        | 2.57                     | 0.46              |
| 2:P:457:PRO:O      | 2:P:458:ALA:HB3     | 2.16                     | 0.46              |
| 1:A:31:PRO:HB2     | 1:A:423:ILE:HD13    | 1.98                     | 0.46              |
| 1:C:316:CYS:N      | 1:C:503:GLN:HE22    | 2.13                     | 0.46              |
| 1:C:381:PRO:HB2    | 9:C:1104:HOH:O      | 2.15                     | 0.46              |
| 1:C:637:ASP:OD1    | 1:C:640:VAL:HG23    | 2.16                     | 0.46              |
| 2:M:395:MET:C      | 2:M:396:GLN:HG3     | 2.41                     | 0.46              |
| 2:N:64:VAL:HG13    | 2:N:111:GLU:OE2     | 2.16                     | 0.46              |
| 2:O:158:ILE:HG22   | 2:O:252:VAL:HG13    | 1.97                     | 0.46              |
| 2:O:247:ARG:O      | 2:O:512:PHE:CZ      | 2.69                     | 0.46              |
| 2:P:95:ASN:O       | 2:P:96:PHE:C        | 2.59                     | 0.46              |
| 2:P:609:ASN:OD1    | 2:P:728:ILE:HG22    | 2.15                     | 0.46              |
| 2:P:674:LEU:O      | 2:P:674:LEU:HD22    | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:466:LEU:HA   | 1:B:496:VAL:HG23 | 1.98                     | 0.46              |
| 2:O:58:THR:HA    | 2:O:138:ASP:OD2  | 2.16                     | 0.46              |
| 2:O:95:ASN:ND2   | 2:O:98:ASN:H     | 2.13                     | 0.46              |
| 2:P:61:TYR:CD2   | 2:P:66:ARG:HD2   | 2.48                     | 0.46              |
| 2:P:344:GLY:O    | 2:P:346:ARG:CZ   | 2.64                     | 0.46              |
| 1:A:118:ASN:C    | 1:A:118:ASN:HD22 | 2.23                     | 0.45              |
| 1:A:584:MET:HG3  | 1:B:73:ALA:HB2   | 1.96                     | 0.45              |
| 1:D:9:HIS:C      | 1:D:9:HIS:CD2    | 2.93                     | 0.45              |
| 2:M:21:LEU:HB2   | 2:M:286:LYS:HA   | 1.97                     | 0.45              |
| 2:N:61:TYR:HD2   | 2:N:66:ARG:HD2   | 1.82                     | 0.45              |
| 2:O:167:LYS:HD3  | 2:O:196:GLU:OE2  | 2.16                     | 0.45              |
| 2:O:266:ALA:O    | 2:O:269:ALA:N    | 2.46                     | 0.45              |
| 2:O:346:ARG:HB3  | 2:O:381:LYS:HD3  | 1.98                     | 0.45              |
| 2:P:456:PHE:O    | 2:P:459:ILE:HB   | 2.15                     | 0.45              |
| 1:A:287:LEU:HB3  | 9:A:1020:HOH:O   | 2.15                     | 0.45              |
| 1:B:9:HIS:CE1    | 1:B:644:LYS:HB3  | 2.51                     | 0.45              |
| 1:B:432:SER:HA   | 1:B:555:ARG:HD3  | 1.98                     | 0.45              |
| 1:B:580:ALA:CB   | 5:B:1001:XE:XE   | 3.39                     | 0.45              |
| 1:B:602:THR:HG23 | 5:B:1001:XE:XE   | 2.94                     | 0.45              |
| 1:D:61:ILE:HG23  | 1:D:66:ILE:HD12  | 1.98                     | 0.45              |
| 1:D:249:THR:O    | 1:D:250:ASP:C    | 2.58                     | 0.45              |
| 2:N:189:ALA:HA   | 2:N:192:GLN:HE21 | 1.80                     | 0.45              |
| 2:O:611:ILE:O    | 2:O:668:VAL:HG22 | 2.16                     | 0.45              |
| 2:O:627:THR:O    | 2:O:628:PHE:C    | 2.58                     | 0.45              |
| 2:P:79:LEU:O     | 2:P:80:PRO:C     | 2.59                     | 0.45              |
| 2:P:538:ALA:O    | 2:P:542:ILE:HG23 | 2.16                     | 0.45              |
| 1:C:105:MET:CE   | 1:C:609:PRO:HD3  | 2.42                     | 0.45              |
| 1:C:256:PHE:CG   | 1:C:289:GLU:HG3  | 2.52                     | 0.45              |
| 1:D:186:LEU:O    | 1:D:190:ILE:HG23 | 2.16                     | 0.45              |
| 2:O:151:TRP:HA   | 2:O:151:TRP:CE3  | 2.51                     | 0.45              |
| 2:O:216:VAL:O    | 2:O:219:ALA:HB3  | 2.16                     | 0.45              |
| 2:O:505:SER:CB   | 2:O:570:TYR:HE2  | 2.28                     | 0.45              |
| 2:O:609:ASN:O    | 2:O:666:ARG:NH1  | 2.50                     | 0.45              |
| 2:P:344:GLY:O    | 2:P:346:ARG:NH1  | 2.50                     | 0.45              |
| 1:A:338:GLU:OE2  | 1:A:359:SER:OG   | 2.30                     | 0.45              |
| 1:A:569:VAL:HA   | 1:A:672:GLN:HE22 | 1.81                     | 0.45              |
| 1:C:531:LEU:HD23 | 1:C:531:LEU:HA   | 1.53                     | 0.45              |
| 1:C:569:VAL:HB   | 1:C:573:LYS:HD3  | 1.98                     | 0.45              |
| 2:M:261:VAL:CG1  | 5:M:1006:XE:XE   | 3.42                     | 0.45              |
| 2:M:657:PHE:O    | 2:M:663:GLY:HA2  | 2.17                     | 0.45              |
| 2:N:367:GLU:HB2  | 9:N:1171:HOH:O   | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:144:PHE:HB3  | 2:O:153:ILE:HD11 | 1.97                     | 0.45              |
| 2:O:639:THR:O    | 2:O:640:GLN:C    | 2.58                     | 0.45              |
| 2:P:439:PHE:O    | 2:P:440:ARG:HD2  | 2.16                     | 0.45              |
| 1:B:386:ILE:HD11 | 1:B:403:MET:CE   | 2.47                     | 0.45              |
| 1:C:288:SER:O    | 1:C:292:VAL:HG23 | 2.15                     | 0.45              |
| 1:C:587:LYS:NZ   | 4:C:800:XCC:S4   | 2.85                     | 0.45              |
| 1:D:545:PHE:N    | 1:D:545:PHE:CD1  | 2.84                     | 0.45              |
| 2:M:373:ILE:HG21 | 2:M:440:ARG:HA   | 1.99                     | 0.45              |
| 1:B:370:ARG:HH11 | 1:B:370:ARG:HG2  | 1.81                     | 0.45              |
| 1:B:601:PRO:HD3  | 1:B:652:ARG:CZ   | 2.47                     | 0.45              |
| 2:O:183:LEU:HA   | 2:O:183:LEU:HD23 | 1.71                     | 0.45              |
| 2:O:439:PHE:CG   | 2:O:440:ARG:N    | 2.84                     | 0.45              |
| 2:O:524:ARG:NH2  | 2:O:645:MET:HE1  | 2.31                     | 0.45              |
| 2:O:590:ASN:C    | 2:O:640:GLN:HE21 | 2.25                     | 0.45              |
| 2:P:150:ASP:OD1  | 2:P:150:ASP:C    | 2.57                     | 0.45              |
| 2:P:611:ILE:O    | 2:P:668:VAL:HG22 | 2.16                     | 0.45              |
| 1:B:308:LYS:HA   | 1:B:308:LYS:HD3  | 1.57                     | 0.45              |
| 1:C:552:ASP:C    | 1:C:554:SER:N    | 2.74                     | 0.45              |
| 2:N:694:ASP:O    | 2:N:695:PHE:C    | 2.59                     | 0.45              |
| 2:O:308:THR:O    | 2:O:309:ARG:C    | 2.58                     | 0.45              |
| 2:O:346:ARG:HH22 | 2:O:427:TRP:HZ2  | 1.64                     | 0.45              |
| 1:D:32:ALA:CB    | 1:D:268:MET:HG3  | 2.45                     | 0.45              |
| 1:D:530:ARG:HH11 | 1:D:530:ARG:CG   | 2.30                     | 0.45              |
| 1:D:572:PRO:O    | 1:D:652:ARG:CZ   | 2.65                     | 0.45              |
| 1:D:600:VAL:HA   | 1:D:601:PRO:HD3  | 1.89                     | 0.45              |
| 2:N:254:TYR:O    | 2:N:278:THR:HA   | 2.17                     | 0.45              |
| 2:N:354:ARG:HB3  | 2:N:484:LYS:HE2  | 1.98                     | 0.45              |
| 2:O:316:ILE:O    | 2:O:316:ILE:CG2  | 2.64                     | 0.45              |
| 2:O:590:ASN:OD1  | 2:O:640:GLN:NE2  | 2.50                     | 0.45              |
| 2:P:369:ILE:HG21 | 2:P:468:PHE:HD2  | 1.82                     | 0.45              |
| 2:P:665:ALA:O    | 2:P:720:HIS:CE1  | 2.70                     | 0.45              |
| 1:C:154:VAL:O    | 1:C:154:VAL:HG12 | 2.17                     | 0.45              |
| 1:C:241:ASP:OD1  | 1:C:245:GLU:OE2  | 2.34                     | 0.45              |
| 1:D:219:ALA:O    | 1:D:220:HIS:C    | 2.58                     | 0.45              |
| 1:D:241:ASP:OD1  | 1:D:245:GLU:OE2  | 2.34                     | 0.45              |
| 1:D:614:ASP:H    | 6:D:863:GOL:H32  | 1.82                     | 0.45              |
| 2:O:534:LEU:O    | 2:O:537:LYS:HB3  | 2.16                     | 0.45              |
| 2:P:212:PHE:O    | 2:P:215:ILE:HG22 | 2.17                     | 0.45              |
| 1:D:138:LYS:HG3  | 1:D:255:LEU:O    | 2.17                     | 0.45              |
| 1:D:287:LEU:HD13 | 1:D:388:TYR:CE1  | 2.51                     | 0.45              |
| 2:M:551:ILE:HG21 | 2:M:567:VAL:HG22 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:79:LEU:HD22  | 2:N:112:ILE:HG12 | 1.99                     | 0.45              |
| 2:P:488:ARG:HG2  | 2:P:491:ARG:HH22 | 1.82                     | 0.45              |
| 2:M:95:ASN:ND2   | 2:M:95:ASN:C     | 2.74                     | 0.44              |
| 2:O:483:GLU:HA   | 2:O:486:LYS:HB2  | 1.99                     | 0.44              |
| 2:O:675:LYS:CA   | 2:O:696:ILE:HD11 | 2.46                     | 0.44              |
| 2:P:342:MET:HE2  | 2:P:384:LEU:HD13 | 2.00                     | 0.44              |
| 1:C:316:CYS:SG   | 4:C:800:XCC:S3   | 3.11                     | 0.44              |
| 1:D:82:ASP:CG    | 1:D:83:GLY:N     | 2.75                     | 0.44              |
| 1:D:105:MET:H    | 1:D:105:MET:HG2  | 1.56                     | 0.44              |
| 2:M:621:MET:CE   | 9:M:1140:HOH:O   | 2.65                     | 0.44              |
| 2:M:621:MET:CE   | 2:M:625:GLY:HA2  | 2.37                     | 0.44              |
| 2:N:389:ASP:HB2  | 2:N:464:GLN:HB3  | 1.99                     | 0.44              |
| 2:O:598:PHE:CE1  | 2:O:601:ILE:HD11 | 2.52                     | 0.44              |
| 2:P:309:ARG:HB3  | 2:P:311:ILE:HG13 | 1.99                     | 0.44              |
| 2:P:723:LEU:HD23 | 2:P:723:LEU:HA   | 1.50                     | 0.44              |
| 1:B:380:ILE:HG22 | 1:B:381:PRO:O    | 2.18                     | 0.44              |
| 2:N:622:THR:HB   | 2:N:623:PRO:HD2  | 1.99                     | 0.44              |
| 2:P:326:PRO:O    | 2:P:327:ALA:C    | 2.58                     | 0.44              |
| 2:P:352:LEU:HG   | 2:P:353:VAL:N    | 2.33                     | 0.44              |
| 2:P:474:VAL:HG13 | 2:P:475:LYS:HG3  | 2.00                     | 0.44              |
| 2:P:604:ILE:O    | 2:P:605:LEU:HD13 | 2.17                     | 0.44              |
| 2:P:605:LEU:HD12 | 2:P:605:LEU:HA   | 1.75                     | 0.44              |
| 1:A:89:ILE:HG12  | 1:B:52:PHE:HA    | 1.99                     | 0.44              |
| 1:A:220:HIS:CE1  | 1:B:587:LYS:HG3  | 2.51                     | 0.44              |
| 1:C:114:CYS:CA   | 9:C:1089:HOH:O   | 2.63                     | 0.44              |
| 2:P:655:LYS:HA   | 2:P:685:ARG:HH12 | 1.82                     | 0.44              |
| 1:A:218:GLN:HE22 | 1:A:233:SER:CB   | 2.30                     | 0.44              |
| 1:B:18:ARG:HH21  | 6:B:861:GOL:H2   | 1.83                     | 0.44              |
| 1:D:552:ASP:O    | 1:D:555:ARG:HB2  | 2.17                     | 0.44              |
| 1:D:620:LEU:CD2  | 5:D:1004:XE:XE   | 3.43                     | 0.44              |
| 2:N:327:ALA:HB2  | 9:N:1172:HOH:O   | 2.17                     | 0.44              |
| 2:O:431:SER:C    | 2:O:433:ASP:N    | 2.76                     | 0.44              |
| 1:A:549:SER:N    | 1:A:552:ASP:HB2  | 2.32                     | 0.44              |
| 1:C:470:CYS:SG   | 1:C:588:ALA:HB2  | 2.58                     | 0.44              |
| 1:D:431:TRP:O    | 1:D:547:MET:HG2  | 2.18                     | 0.44              |
| 2:M:114:GLU:O    | 2:M:115:ALA:C    | 2.57                     | 0.44              |
| 2:N:229:PHE:CE1  | 5:N:1009:XE:XE   | 3.49                     | 0.44              |
| 2:O:169:LEU:CD1  | 2:O:193:LEU:HG   | 2.48                     | 0.44              |
| 2:O:641:THR:O    | 2:O:642:PRO:C    | 2.61                     | 0.44              |
| 2:P:138:ASP:N    | 2:P:139:PRO:CD   | 2.81                     | 0.44              |
| 2:P:657:PHE:CE2  | 2:P:667:ILE:HD11 | 2.53                     | 0.44              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:A:27:ARG:CZ      | 1:A:27:ARG:HB3   | 2.48                     | 0.44              |
| 1:A:137:VAL:HG13   | 1:A:254:ILE:HG23 | 1.99                     | 0.44              |
| 1:A:226:ASP:C      | 1:A:226:ASP:OD1  | 2.61                     | 0.44              |
| 1:B:587:LYS:NZ     | 4:B:800:XCC:S4   | 2.91                     | 0.44              |
| 2:N:626:MET:HB3    | 2:N:630:THR:HB   | 1.99                     | 0.44              |
| 2:O:191:GLU:O      | 2:O:195:GLU:HB2  | 2.18                     | 0.44              |
| 2:O:622:THR:OG1    | 2:O:626:MET:O    | 2.29                     | 0.44              |
| 2:P:373:ILE:HD13   | 2:P:435:VAL:CG2  | 2.47                     | 0.44              |
| 1:B:384:TYR:HD2    | 1:B:403:MET:SD   | 2.41                     | 0.44              |
| 1:B:537:ILE:C      | 1:B:539:ILE:H    | 2.25                     | 0.44              |
| 1:C:650:GLU:HA     | 1:C:653:THR:OG1  | 2.18                     | 0.44              |
| 1:D:285:PRO:C      | 1:D:287:LEU:H    | 2.24                     | 0.44              |
| 2:M:424:ASN:N      | 2:M:424:ASN:ND2  | 2.66                     | 0.44              |
| 2:N:185:ILE:HD12   | 2:N:185:ILE:N    | 2.33                     | 0.44              |
| 2:O:174:LYS:HA     | 9:O:1030:HOH:O   | 2.17                     | 0.44              |
| 2:P:371:PRO:HD2    | 2:P:469:THR:HB   | 1.99                     | 0.44              |
| 2:P:585:TYR:O      | 2:P:658:ILE:HA   | 2.17                     | 0.44              |
| 1:D:636:MET:HE2    | 9:D:1043:HOH:O   | 2.18                     | 0.44              |
| 2:N:621:MET:HE1    | 2:N:622:THR:O    | 2.18                     | 0.44              |
| 2:O:491:ARG:HH11   | 2:O:491:ARG:CB   | 2.30                     | 0.44              |
| 2:O:572:TYR:CE2    | 2:O:577:ARG:HB3  | 2.53                     | 0.44              |
| 2:P:354:ARG:O      | 2:P:390:ILE:HG22 | 2.18                     | 0.44              |
| 1:B:537:ILE:HD13   | 1:B:537:ILE:HA   | 1.94                     | 0.43              |
| 1:C:287:LEU:HB3    | 9:C:1118:HOH:O   | 2.17                     | 0.43              |
| 1:D:66:ILE:H       | 1:D:66:ILE:HG13  | 1.65                     | 0.43              |
| 2:N:58:THR:HA      | 2:N:138:ASP:CG   | 2.43                     | 0.43              |
| 2:O:6:LYS:O        | 2:O:9:GLU:HB2    | 2.18                     | 0.43              |
| 2:O:180:GLY:HA2    | 2:O:326:PRO:CG   | 2.48                     | 0.43              |
| 2:O:356:VAL:HG23   | 2:O:361:ILE:HD12 | 2.00                     | 0.43              |
| 2:O:720:HIS:C      | 2:O:722:ALA:H    | 2.26                     | 0.43              |
| 2:P:674:LEU:HD13   | 2:P:678:LEU:HD11 | 2.00                     | 0.43              |
| 1:A:342:CYS:HA     | 1:A:367:TYR:CZ   | 2.53                     | 0.43              |
| 1:B:283:HIS:CD2    | 1:B:317:CYS:HB2  | 2.53                     | 0.43              |
| 1:D:607:MET:HG3    | 1:D:608:PRO:O    | 2.18                     | 0.43              |
| 1:D:615:LEU:H      | 6:D:863:GOL:H11  | 1.83                     | 0.43              |
| 2:N:558:ASP:OD1    | 2:N:560:ILE:N    | 2.51                     | 0.43              |
| 2:O:193:LEU:O      | 2:O:198:VAL:HG13 | 2.18                     | 0.43              |
| 2:P:3:ASP:O        | 2:P:6:LYS:HB3    | 2.18                     | 0.43              |
| 1:A:9:HIS:CD2      | 1:A:9:HIS:C      | 2.96                     | 0.43              |
| 1:B:114[A]:CYS:HB3 | 1:B:208:ILE:HG21 | 1.99                     | 0.43              |
| 1:D:261:PRO:HA     | 1:D:429:ALA:O    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:604:ILE:HG23 | 2:M:611:ILE:HG22 | 2.01                     | 0.43              |
| 2:N:384:LEU:HA   | 2:N:468:PHE:O    | 2.18                     | 0.43              |
| 2:O:361:ILE:HD13 | 2:O:391:TYR:CB   | 2.46                     | 0.43              |
| 2:P:613:ILE:HD13 | 2:P:652:ILE:HG12 | 1.99                     | 0.43              |
| 1:A:220:HIS:CD2  | 1:A:221:MET:O    | 2.71                     | 0.43              |
| 1:A:567:LEU:HD12 | 1:A:574:VAL:HG22 | 2.01                     | 0.43              |
| 1:B:18:ARG:HD2   | 1:B:636:MET:HE3  | 2.00                     | 0.43              |
| 1:B:287:LEU:HD12 | 1:B:388:TYR:CE1  | 2.54                     | 0.43              |
| 1:D:322:VAL:O    | 1:D:326:GLN:HB2  | 2.18                     | 0.43              |
| 2:N:478:MET:HG3  | 2:N:478:MET:O    | 2.18                     | 0.43              |
| 2:O:142:ARG:NH1  | 2:O:228:MET:HG2  | 2.33                     | 0.43              |
| 2:O:603:ALA:O    | 2:O:604:ILE:C    | 2.60                     | 0.43              |
| 2:P:541:GLU:H    | 2:P:541:GLU:HG2  | 1.54                     | 0.43              |
| 1:B:483:THR:HB   | 1:B:638:PRO:HB2  | 2.01                     | 0.43              |
| 1:B:525:LYS:O    | 1:B:526:GLY:C    | 2.61                     | 0.43              |
| 1:C:280:LEU:HD23 | 1:C:280:LEU:HA   | 1.74                     | 0.43              |
| 1:D:217:ASN:O    | 1:D:223:MET:HG3  | 2.18                     | 0.43              |
| 1:D:531:LEU:HD23 | 1:D:531:LEU:HA   | 1.75                     | 0.43              |
| 2:N:315:LYS:CE   | 9:N:1162:HOH:O   | 2.67                     | 0.43              |
| 2:O:491:ARG:O    | 2:O:495:LEU:HB2  | 2.19                     | 0.43              |
| 2:P:558:ASP:OD1  | 2:P:558:ASP:C    | 2.62                     | 0.43              |
| 1:A:238:ALA:O    | 1:A:241:ASP:HB3  | 2.19                     | 0.43              |
| 1:C:223:MET:HG2  | 1:D:354:GLN:HA   | 2.01                     | 0.43              |
| 1:C:559:LEU:O    | 1:C:563:MET:HG3  | 2.18                     | 0.43              |
| 2:N:51:HIS:HB3   | 2:N:76:LEU:HD12  | 2.01                     | 0.43              |
| 2:O:334:ARG:NH1  | 2:O:335:LYS:CG   | 2.82                     | 0.43              |
| 2:P:369:ILE:HG21 | 2:P:468:PHE:CD2  | 2.54                     | 0.43              |
| 2:P:479:GLU:O    | 2:P:480:VAL:C    | 2.61                     | 0.43              |
| 1:A:394:ILE:HD12 | 1:A:394:ILE:HA   | 1.75                     | 0.43              |
| 1:B:47:THR:HB    | 1:B:338:GLU:OE1  | 2.19                     | 0.43              |
| 1:B:298:MET:HE2  | 1:B:301:GLU:OE2  | 2.18                     | 0.43              |
| 1:C:626:ASP:HB3  | 2:O:212:PHE:CG   | 2.53                     | 0.43              |
| 2:M:335:LYS:HG3  | 2:M:429:ARG:HH22 | 1.83                     | 0.43              |
| 2:O:608:CYS:SG   | 2:O:712:LEU:HD12 | 2.58                     | 0.43              |
| 1:A:283:HIS:CE1  | 4:A:800:XCC:S3   | 3.11                     | 0.43              |
| 1:A:426:ARG:HH22 | 1:A:539:ILE:HB   | 1.82                     | 0.43              |
| 1:B:484:VAL:O    | 1:B:488:LEU:HG   | 2.19                     | 0.43              |
| 1:C:281:HIS:O    | 1:C:351:VAL:HA   | 2.18                     | 0.43              |
| 1:C:436:LEU:HD23 | 1:C:436:LEU:HA   | 1.74                     | 0.43              |
| 1:D:637:ASP:OD1  | 1:D:637:ASP:C    | 2.62                     | 0.43              |
| 2:N:85:ARG:HD2   | 9:N:1043:HOH:O   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:423:ARG:HB3  | 2:N:485:TYR:CE2  | 2.53                     | 0.43              |
| 2:N:674:LEU:HD22 | 2:N:678:LEU:HG   | 2.00                     | 0.43              |
| 2:P:358:GLU:HA   | 2:P:361:ILE:CG2  | 2.49                     | 0.43              |
| 2:P:412:ASN:HD21 | 2:P:419:HIS:HB3  | 1.82                     | 0.43              |
| 2:P:626:MET:HE3  | 2:P:631:LEU:HD13 | 2.00                     | 0.43              |
| 1:C:87:ARG:HD3   | 1:C:91:GLY:O     | 2.19                     | 0.43              |
| 2:M:419:HIS:HE1  | 2:M:421:GLY:O    | 2.02                     | 0.43              |
| 2:M:427:TRP:C    | 2:M:428:LEU:HD12 | 2.42                     | 0.43              |
| 2:M:428:LEU:N    | 2:M:428:LEU:CD1  | 2.81                     | 0.43              |
| 2:O:263:THR:O    | 2:O:266:ALA:HB3  | 2.19                     | 0.43              |
| 2:O:569:ASP:O    | 2:O:573:THR:HG23 | 2.18                     | 0.43              |
| 2:P:199:LYS:HG2  | 2:P:204:TYR:CZ   | 2.54                     | 0.43              |
| 2:P:256:GLY:O    | 2:P:257:GLU:C    | 2.61                     | 0.43              |
| 1:A:549:SER:O    | 1:A:552:ASP:HB2  | 2.19                     | 0.43              |
| 1:B:280:LEU:HD13 | 1:B:288:SER:HB2  | 2.01                     | 0.43              |
| 1:D:124:LEU:HD12 | 1:D:255:LEU:HD21 | 2.00                     | 0.43              |
| 2:O:508:LEU:C    | 2:O:510:GLN:N    | 2.76                     | 0.43              |
| 2:P:378:GLU:O    | 2:P:380:SER:N    | 2.52                     | 0.43              |
| 2:P:426:ASN:O    | 2:P:427:TRP:CB   | 2.67                     | 0.43              |
| 1:A:110:ALA:HA   | 1:A:241:ASP:OD2  | 2.19                     | 0.42              |
| 1:A:470:CYS:HB3  | 4:A:800:XCC:S2   | 2.59                     | 0.42              |
| 1:B:18:ARG:CD    | 1:B:636:MET:HE3  | 2.48                     | 0.42              |
| 1:B:50:ASP:OD2   | 9:B:1055:HOH:O   | 2.21                     | 0.42              |
| 1:B:317:CYS:HB3  | 9:B:1019:HOH:O   | 2.19                     | 0.42              |
| 1:D:279:VAL:CG1  | 1:D:315:ILE:CD1  | 2.84                     | 0.42              |
| 2:M:55:TYR:HB3   | 2:M:56:PRO:HD2   | 2.00                     | 0.42              |
| 2:M:623:PRO:HA   | 2:M:707:THR:HA   | 2.01                     | 0.42              |
| 2:N:160:LEU:HD21 | 2:N:262:LYS:HG2  | 2.01                     | 0.42              |
| 2:N:316:ILE:HD13 | 2:N:317:LYS:O    | 2.19                     | 0.42              |
| 2:O:527:LEU:HA   | 2:O:648:GLY:H    | 1.84                     | 0.42              |
| 2:P:182:MET:HB2  | 2:P:205:ILE:HG22 | 2.00                     | 0.42              |
| 1:A:186:LEU:HD22 | 1:A:205:PRO:HD2  | 2.00                     | 0.42              |
| 1:A:574:VAL:O    | 1:A:576:PHE:N    | 2.51                     | 0.42              |
| 1:D:285:PRO:O    | 1:D:286:LEU:C    | 2.61                     | 0.42              |
| 2:M:604:ILE:HG22 | 2:M:610:GLY:O    | 2.19                     | 0.42              |
| 2:O:409:ASP:O    | 2:O:410:PHE:C    | 2.62                     | 0.42              |
| 2:O:509:CYS:CB   | 2:O:595:CYS:SG   | 3.07                     | 0.42              |
| 2:P:492:MET:O    | 2:P:493:ARG:C    | 2.63                     | 0.42              |
| 1:B:268:MET:HA   | 1:B:331:VAL:HG23 | 2.01                     | 0.42              |
| 1:B:287:LEU:HA   | 1:B:388:TYR:CZ   | 2.55                     | 0.42              |
| 1:C:209:HIS:CD2  | 1:D:213:SER:OG   | 2.69                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:N:382:LEU:HD12   | 2:N:382:LEU:HA    | 1.88                     | 0.42              |
| 2:N:439:PHE:CD2    | 2:N:439:PHE:C     | 2.97                     | 0.42              |
| 2:O:79:LEU:N       | 2:O:80:PRO:CD     | 2.82                     | 0.42              |
| 2:O:160:LEU:HD13   | 2:O:215:ILE:HD13  | 2.02                     | 0.42              |
| 2:O:356:VAL:HG11   | 2:O:360:GLU:CD    | 2.45                     | 0.42              |
| 2:P:448:LEU:O      | 2:P:452:MET:HG2   | 2.20                     | 0.42              |
| 1:A:453:ASN:ND2    | 1:A:566:ASP:HB3   | 2.34                     | 0.42              |
| 1:B:467:ILE:O      | 1:B:497:ALA:HA    | 2.19                     | 0.42              |
| 1:C:574:VAL:O      | 1:C:576:PHE:N     | 2.50                     | 0.42              |
| 1:D:134:ASP:HB3    | 1:D:290:ILE:HD12  | 2.00                     | 0.42              |
| 2:M:592:MET:HE3    | 2:M:592:MET:HB2   | 1.92                     | 0.42              |
| 2:N:66:ARG:HD3     | 9:N:1029:HOH:O    | 2.19                     | 0.42              |
| 2:O:174:LYS:HE2    | 2:O:323:ASN:ND2   | 2.34                     | 0.42              |
| 2:O:430:VAL:HG12   | 2:O:434:ALA:HB3   | 2.01                     | 0.42              |
| 2:O:468:PHE:HB2    | 2:O:474:VAL:CG2   | 2.41                     | 0.42              |
| 2:P:315[A]:LYS:HD3 | 9:P:1080:HOH:O    | 2.19                     | 0.42              |
| 2:P:323:ASN:HB2    | 2:P:415:GLU:OE1   | 2.19                     | 0.42              |
| 2:P:359:SER:C      | 2:P:361:ILE:H     | 2.27                     | 0.42              |
| 1:A:2:PRO:N        | 6:A:862:GOL:O1    | 2.52                     | 0.42              |
| 1:A:162:LEU:HD23   | 1:A:162:LEU:HA    | 1.72                     | 0.42              |
| 1:B:579:SER:HA     | 1:B:603:HIS:O     | 2.20                     | 0.42              |
| 1:B:602:THR:CG2    | 5:B:1001:XE:XE    | 3.46                     | 0.42              |
| 1:C:190:ILE:HG13   | 1:C:195:LYS:HG3   | 2.01                     | 0.42              |
| 1:D:592:GLY:HA2    | 5:D:1001:XE:XE    | 2.98                     | 0.42              |
| 2:M:448:LEU:HD12   | 2:M:448:LEU:HA    | 1.90                     | 0.42              |
| 2:M:503:PHE:CG     | 2:M:521:THR:HG22  | 2.54                     | 0.42              |
| 2:N:466:THR:HG21   | 2:N:468:PHE:CZ    | 2.55                     | 0.42              |
| 2:O:114:GLU:HG3    | 2:O:216:VAL:HG12  | 2.01                     | 0.42              |
| 2:O:397:ALA:HA     | 2:O:400:GLU:HG3   | 2.01                     | 0.42              |
| 2:P:722:ALA:HA     | 2:P:725:MET:SD    | 2.60                     | 0.42              |
| 1:A:6:ASP:OD1      | 1:A:6:ASP:C       | 2.63                     | 0.42              |
| 1:A:106:ILE:HD11   | 5:A:1003[A]:XE:XE | 2.98                     | 0.42              |
| 1:A:515:ASN:HA     | 1:A:518:THR:HG23  | 2.02                     | 0.42              |
| 1:D:292:VAL:HG22   | 1:D:312:LEU:HD13  | 2.01                     | 0.42              |
| 1:D:400:ALA:HB2    | 5:D:1010:XE:XE    | 2.98                     | 0.42              |
| 2:N:107:TRP:CZ3    | 2:N:219:ALA:HB1   | 2.54                     | 0.42              |
| 2:N:405:ARG:HD2    | 9:N:1219:HOH:O    | 2.18                     | 0.42              |
| 2:O:470:ASP:O      | 2:O:474:VAL:HB    | 2.19                     | 0.42              |
| 2:P:528:CYS:HB3    | 3:P:900:SF4:S3    | 2.59                     | 0.42              |
| 2:P:668:VAL:HB     | 2:P:715:LEU:HD11  | 2.01                     | 0.42              |
| 1:A:338:GLU:HB2    | 9:A:1023:HOH:O    | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:637:ASP:HA   | 1:B:638:PRO:HD2  | 1.75                     | 0.42              |
| 1:C:655:LYS:NZ   | 1:C:674:TYR:O    | 2.38                     | 0.42              |
| 2:M:121:TYR:CD1  | 2:M:121:TYR:C    | 2.98                     | 0.42              |
| 2:M:525:VAL:HG23 | 2:M:532:SER:HA   | 2.01                     | 0.42              |
| 2:N:199:LYS:HD2  | 2:N:204:TYR:CE2  | 2.55                     | 0.42              |
| 2:N:478:MET:O    | 2:N:482:ARG:HG3  | 2.20                     | 0.42              |
| 2:O:182:MET:HG3  | 2:O:205:ILE:HG22 | 2.01                     | 0.42              |
| 2:O:482:ARG:HH12 | 2:O:485:TYR:HE1  | 1.67                     | 0.42              |
| 2:O:497:ASP:HB2  | 2:O:656:LYS:HZ1  | 1.84                     | 0.42              |
| 2:O:669:TRP:CD1  | 2:O:711:ILE:HG21 | 2.53                     | 0.42              |
| 2:P:184:PHE:HD1  | 2:P:209:LEU:HD21 | 1.84                     | 0.42              |
| 2:P:392:GLY:H    | 2:P:395:MET:HB2  | 1.84                     | 0.42              |
| 1:A:2:PRO:HB2    | 1:A:651:TYR:CE2  | 2.55                     | 0.42              |
| 1:B:287:LEU:HD13 | 1:B:388:TYR:CD1  | 2.54                     | 0.42              |
| 1:B:572:PRO:CG   | 1:B:629:GLY:HA3  | 2.50                     | 0.42              |
| 1:C:283:HIS:CD2  | 1:C:317:CYS:CB   | 3.00                     | 0.42              |
| 2:N:26:TYR:CE1   | 2:N:30:ILE:HD11  | 2.55                     | 0.42              |
| 2:N:150:ASP:OD1  | 2:N:150:ASP:C    | 2.59                     | 0.42              |
| 2:N:243:TYR:CZ   | 2:N:247:ARG:HD3  | 2.54                     | 0.42              |
| 2:O:118:TYR:CE2  | 2:O:121:TYR:CD2  | 3.08                     | 0.42              |
| 1:B:536:ASN:HD22 | 1:C:23:LYS:HB3   | 1.85                     | 0.42              |
| 1:C:154:VAL:O    | 1:C:154:VAL:CG1  | 2.67                     | 0.42              |
| 1:C:187:MET:HE3  | 1:C:195:LYS:HG2  | 2.02                     | 0.42              |
| 1:D:215:LEU:HD22 | 1:D:234:ALA:HA   | 2.02                     | 0.42              |
| 1:D:324:MET:HE3  | 1:D:324:MET:HB3  | 1.95                     | 0.42              |
| 1:D:496:VAL:HG11 | 1:D:547:MET:SD   | 2.60                     | 0.42              |
| 2:M:64:VAL:HB    | 2:M:223:LEU:HD12 | 2.02                     | 0.42              |
| 2:O:278:THR:O    | 2:O:294:SER:HA   | 2.20                     | 0.42              |
| 2:P:316:ILE:HD13 | 2:P:454:GLU:CD   | 2.45                     | 0.42              |
| 1:A:105:MET:HE3  | 1:A:105:MET:HB3  | 1.86                     | 0.42              |
| 1:A:414:SER:O    | 1:A:416:ARG:HD2  | 2.19                     | 0.42              |
| 1:A:577:VAL:HG13 | 1:A:649:LEU:CD2  | 2.50                     | 0.42              |
| 1:B:637:ASP:OD1  | 1:B:637:ASP:C    | 2.63                     | 0.42              |
| 1:D:287:LEU:HA   | 1:D:388:TYR:OH   | 2.19                     | 0.42              |
| 2:M:152:THR:O    | 2:M:154:PRO:HD3  | 2.20                     | 0.42              |
| 2:O:338:MET:SD   | 2:O:341:GLU:HB2  | 2.60                     | 0.42              |
| 2:O:628:PHE:O    | 2:O:632:ALA:N    | 2.39                     | 0.42              |
| 2:O:712:LEU:HA   | 2:O:715:LEU:HB2  | 2.00                     | 0.42              |
| 2:P:289:PRO:O    | 2:P:290:ASP:HB2  | 2.20                     | 0.42              |
| 2:P:395:MET:SD   | 2:P:459:ILE:HG23 | 2.60                     | 0.42              |
| 1:A:380:ILE:O    | 1:A:381:PRO:C    | 2.61                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:176:ARG:O    | 1:B:207:GLY:HA3   | 2.20                     | 0.41              |
| 1:B:577:VAL:HG13 | 1:B:649:LEU:CD2   | 2.50                     | 0.41              |
| 1:B:620:LEU:HD21 | 5:B:1003[A]:XE:XE | 2.98                     | 0.41              |
| 1:D:353:VAL:O    | 1:D:354:GLN:HB2   | 2.19                     | 0.41              |
| 2:M:16:LYS:HA    | 2:M:16:LYS:HD2    | 1.37                     | 0.41              |
| 2:N:43:ALA:O     | 2:N:47:TYR:HD2    | 2.03                     | 0.41              |
| 2:O:121:TYR:CD1  | 2:O:121:TYR:C     | 2.98                     | 0.41              |
| 2:O:504:TYR:HA   | 2:O:549:GLN:O     | 2.20                     | 0.41              |
| 2:O:592:MET:HB2  | 2:O:592:MET:HE3   | 1.61                     | 0.41              |
| 2:O:672:LYS:C    | 2:O:674:LEU:N     | 2.77                     | 0.41              |
| 2:O:675:LYS:H    | 2:O:675:LYS:HG2   | 1.61                     | 0.41              |
| 2:P:349:ALA:C    | 2:P:426:ASN:HD22  | 2.28                     | 0.41              |
| 2:P:392:GLY:C    | 2:P:394:LYS:H     | 2.27                     | 0.41              |
| 1:B:88:GLY:HA3   | 3:B:700:SF4:S3    | 2.60                     | 0.41              |
| 1:C:603:HIS:HA   | 1:C:633:ILE:HB    | 2.01                     | 0.41              |
| 2:M:357:SER:O    | 2:M:360:GLU:HB2   | 2.20                     | 0.41              |
| 2:N:349:ALA:HA   | 2:N:384:LEU:O     | 2.20                     | 0.41              |
| 2:N:549:GLN:NE2  | 2:N:570:TYR:OH    | 2.53                     | 0.41              |
| 2:O:127:LEU:O    | 2:O:128:LEU:HD23  | 2.20                     | 0.41              |
| 2:O:368:VAL:HG22 | 2:O:442:LYS:HB3   | 2.01                     | 0.41              |
| 2:P:369:ILE:HG23 | 2:P:370:GLY:N     | 2.36                     | 0.41              |
| 2:P:481:ALA:HB1  | 2:P:485:TYR:CZ    | 2.55                     | 0.41              |
| 1:A:213:SER:CB   | 1:B:209:HIS:HD2   | 2.33                     | 0.41              |
| 1:D:28:THR:HG21  | 1:D:33:VAL:CG1    | 2.51                     | 0.41              |
| 2:O:500:VAL:HG22 | 2:O:501:ASP:H     | 1.85                     | 0.41              |
| 2:P:351:GLU:O    | 2:P:485:TYR:OH    | 2.31                     | 0.41              |
| 1:A:142:LYS:NZ   | 1:A:253:ASP:OD2   | 2.44                     | 0.41              |
| 1:A:607:MET:HG3  | 1:A:608:PRO:O     | 2.21                     | 0.41              |
| 1:B:18:ARG:NE    | 1:B:636:MET:HE3   | 2.34                     | 0.41              |
| 1:C:144:LYS:HG2  | 1:C:154:VAL:HG11  | 2.02                     | 0.41              |
| 2:M:669:TRP:HA   | 2:M:700:ALA:O     | 2.20                     | 0.41              |
| 2:N:615:THR:HG21 | 2:N:674:LEU:HG    | 2.02                     | 0.41              |
| 2:O:335:LYS:HG3  | 2:O:336:GLY:H     | 1.85                     | 0.41              |
| 2:O:683:VAL:O    | 2:O:686:SER:HB2   | 2.21                     | 0.41              |
| 1:A:23:LYS:HE3   | 9:A:1176:HOH:O    | 2.20                     | 0.41              |
| 1:C:348:ALA:HA   | 1:C:370:ARG:O     | 2.21                     | 0.41              |
| 2:M:278:THR:O    | 2:M:294:SER:HA    | 2.21                     | 0.41              |
| 2:N:223:LEU:HD23 | 2:N:223:LEU:HA    | 1.88                     | 0.41              |
| 2:N:243:TYR:CE2  | 2:N:247:ARG:HD3   | 2.56                     | 0.41              |
| 2:P:268:GLY:O    | 2:P:272:THR:HG22  | 2.21                     | 0.41              |
| 1:A:277:ASN:HB2  | 1:A:345:ALA:O     | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:560:LEU:HD22 | 1:A:600:VAL:HG21 | 2.02                     | 0.41              |
| 1:B:574:VAL:HA   | 1:B:575:PRO:HD3  | 1.89                     | 0.41              |
| 1:D:557:VAL:O    | 1:D:558:ASP:C    | 2.64                     | 0.41              |
| 2:N:87:ARG:HD2   | 9:N:1013:HOH:O   | 2.20                     | 0.41              |
| 2:N:314:THR:O    | 2:N:315:LYS:C    | 2.63                     | 0.41              |
| 2:N:403:LEU:O    | 2:N:452:MET:HE1  | 2.19                     | 0.41              |
| 2:O:302:VAL:O    | 2:O:306:MET:HG3  | 2.20                     | 0.41              |
| 2:P:358:GLU:HG3  | 2:P:462:ARG:NH1  | 2.36                     | 0.41              |
| 1:A:125:VAL:HG23 | 1:A:167:GLY:HA3  | 2.02                     | 0.41              |
| 1:A:235:ILE:HD11 | 5:A:1004:XE:XE   | 2.98                     | 0.41              |
| 1:A:603:HIS:HA   | 1:A:633:ILE:O    | 2.20                     | 0.41              |
| 1:B:447:ASN:O    | 1:B:450:ARG:HB3  | 2.21                     | 0.41              |
| 1:C:332:THR:HG23 | 1:C:333:SER:N    | 2.36                     | 0.41              |
| 1:D:573:LYS:HE2  | 1:D:671:CYS:O    | 2.21                     | 0.41              |
| 2:M:463:VAL:HG12 | 2:M:464:GLN:N    | 2.36                     | 0.41              |
| 2:M:606:PRO:O    | 2:M:608:CYS:N    | 2.54                     | 0.41              |
| 2:O:142:ARG:CZ   | 2:O:228:MET:HG2  | 2.50                     | 0.41              |
| 2:O:335:LYS:CD   | 2:O:336:GLY:N    | 2.83                     | 0.41              |
| 2:O:482:ARG:NH1  | 2:O:482:ARG:HA   | 2.35                     | 0.41              |
| 2:O:527:LEU:HD12 | 2:O:528:CYS:N    | 2.36                     | 0.41              |
| 2:P:3:ASP:HB2    | 9:P:1058:HOH:O   | 2.20                     | 0.41              |
| 2:P:393:ARG:HB3  | 2:P:393:ARG:CZ   | 2.49                     | 0.41              |
| 2:P:556:GLU:OE1  | 2:P:559:PRO:HG3  | 2.21                     | 0.41              |
| 2:P:602:MET:HE3  | 2:P:602:MET:HB2  | 1.92                     | 0.41              |
| 1:B:14:SER:O     | 6:B:861:GOL:H12  | 2.21                     | 0.41              |
| 1:B:256:PHE:CG   | 1:B:289:GLU:HG3  | 2.56                     | 0.41              |
| 1:B:353:VAL:O    | 1:B:354:GLN:HB2  | 2.19                     | 0.41              |
| 1:D:416:ARG:C    | 1:D:418:VAL:N    | 2.78                     | 0.41              |
| 2:N:607:GLU:HB3  | 9:N:1067:HOH:O   | 2.21                     | 0.41              |
| 2:N:678:LEU:O    | 2:N:679:HIS:C    | 2.63                     | 0.41              |
| 2:O:340:VAL:HG12 | 2:O:380:SER:O    | 2.19                     | 0.41              |
| 2:O:342:MET:HG3  | 2:O:384:LEU:HD23 | 2.02                     | 0.41              |
| 2:O:396:GLN:HB2  | 2:O:399:PHE:CD2  | 2.55                     | 0.41              |
| 2:O:408:HIS:O    | 2:O:412:ASN:HB2  | 2.21                     | 0.41              |
| 2:P:163:ALA:CB   | 2:P:169:LEU:HB2  | 2.50                     | 0.41              |
| 2:P:424:ASN:ND2  | 2:P:485:TYR:HD2  | 2.19                     | 0.41              |
| 1:A:90:CYS:O     | 1:B:357:MET:HG2  | 2.21                     | 0.41              |
| 1:B:466:LEU:HA   | 1:B:496:VAL:O    | 2.21                     | 0.41              |
| 1:C:439:LEU:HD21 | 1:C:531:LEU:HD13 | 2.03                     | 0.41              |
| 2:M:182:MET:HG3  | 2:M:205:ILE:HG22 | 2.03                     | 0.41              |
| 2:M:309:ARG:HA   | 2:M:309:ARG:HD2  | 1.82                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:651:TYR:O    | 2:M:654:SER:HB3  | 2.21                     | 0.41              |
| 2:N:16:LYS:HE2   | 2:N:16:LYS:HB3   | 1.63                     | 0.41              |
| 2:N:61:TYR:CD2   | 2:N:66:ARG:HD2   | 2.56                     | 0.41              |
| 2:N:245:ARG:HD2  | 9:N:1137:HOH:O   | 2.21                     | 0.41              |
| 2:N:288:ILE:O    | 2:N:289:PRO:C    | 2.64                     | 0.41              |
| 2:N:570:TYR:CD1  | 2:N:570:TYR:C    | 2.98                     | 0.41              |
| 2:O:71:GLU:HG3   | 2:O:82:ILE:CD1   | 2.51                     | 0.41              |
| 2:O:79:LEU:HD22  | 2:O:112:ILE:HG12 | 2.03                     | 0.41              |
| 2:O:151:TRP:HA   | 2:O:151:TRP:HE3  | 1.86                     | 0.41              |
| 2:O:521:THR:O    | 2:O:522:PRO:C    | 2.62                     | 0.41              |
| 2:O:602:MET:HG2  | 2:O:611:ILE:HD12 | 2.03                     | 0.41              |
| 2:P:64:VAL:HB    | 2:P:223:LEU:HD12 | 2.03                     | 0.41              |
| 2:P:147:LYS:NZ   | 2:P:329:GLU:OE1  | 2.54                     | 0.41              |
| 2:P:230:GLY:HA3  | 2:P:243:TYR:CE2  | 2.56                     | 0.41              |
| 2:P:605:LEU:O    | 2:P:606:PRO:C    | 2.63                     | 0.41              |
| 2:P:626:MET:CE   | 2:P:631:LEU:HD13 | 2.50                     | 0.41              |
| 1:A:401:ILE:HG22 | 1:A:405:ILE:HD12 | 2.03                     | 0.41              |
| 1:B:316:CYS:HB3  | 1:B:317:CYS:H    | 1.66                     | 0.41              |
| 1:C:73:ALA:HB2   | 1:D:584:MET:HG3  | 2.03                     | 0.41              |
| 1:C:256:PHE:CD1  | 1:C:289:GLU:HG3  | 2.55                     | 0.41              |
| 1:C:260:GLN:O    | 1:C:261:PRO:C    | 2.64                     | 0.41              |
| 2:N:146:ILE:HG22 | 9:N:1044:HOH:O   | 2.21                     | 0.41              |
| 2:O:111:GLU:HB2  | 2:O:216:VAL:HG21 | 2.02                     | 0.41              |
| 2:O:243:TYR:CE2  | 2:O:247:ARG:HD2  | 2.56                     | 0.41              |
| 2:O:407:ILE:O    | 2:O:410:PHE:N    | 2.54                     | 0.41              |
| 2:P:64:VAL:HG13  | 2:P:111:GLU:CD   | 2.46                     | 0.41              |
| 1:A:655:LYS:NZ   | 1:A:674:TYR:O    | 2.51                     | 0.40              |
| 1:C:316:CYS:HB3  | 1:C:317:CYS:H    | 1.78                     | 0.40              |
| 2:M:282:LEU:HA   | 2:M:283:PRO:HD2  | 1.86                     | 0.40              |
| 2:N:353:VAL:HG22 | 2:N:388:VAL:HB   | 2.02                     | 0.40              |
| 2:N:424:ASN:HD22 | 2:N:425:ILE:N    | 2.19                     | 0.40              |
| 2:O:444:TYR:O    | 2:O:448:LEU:HG   | 2.20                     | 0.40              |
| 2:P:18:PRO:HB2   | 2:P:21:LEU:HB3   | 2.03                     | 0.40              |
| 2:P:316:ILE:HD12 | 2:P:316:ILE:HA   | 1.94                     | 0.40              |
| 1:A:68:CYS:HB2   | 1:A:97:ILE:CG2   | 2.46                     | 0.40              |
| 1:B:127:MET:HA   | 1:B:132:ALA:HB3  | 2.03                     | 0.40              |
| 1:B:299:GLU:O    | 1:B:303:LYS:HG3  | 2.21                     | 0.40              |
| 1:C:261:PRO:HA   | 1:C:429:ALA:O    | 2.21                     | 0.40              |
| 1:D:36:MET:CE    | 1:D:343:THR:HA   | 2.50                     | 0.40              |
| 2:M:67:CYS:SG    | 2:M:223:LEU:HB3  | 2.61                     | 0.40              |
| 2:M:655:LYS:HG2  | 2:M:685:ARG:NH1  | 2.36                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:206:ALA:O    | 2:N:208:PRO:HD3  | 2.21                     | 0.40              |
| 2:N:607:GLU:CB   | 9:N:1067:HOH:O   | 2.69                     | 0.40              |
| 2:O:51:HIS:HA    | 2:O:52:PRO:HD3   | 1.91                     | 0.40              |
| 2:O:343:GLY:O    | 2:O:346:ARG:NH1  | 2.55                     | 0.40              |
| 2:O:602:MET:O    | 2:O:644:PHE:HA   | 2.21                     | 0.40              |
| 2:P:607:GLU:HB3  | 2:P:708:VAL:HG11 | 2.03                     | 0.40              |
| 1:A:2:PRO:HD3    | 1:A:625:SER:CB   | 2.51                     | 0.40              |
| 1:B:218:GLN:HE22 | 1:B:233:SER:CB   | 2.34                     | 0.40              |
| 1:B:576:PHE:C    | 1:B:576:PHE:CD1  | 2.99                     | 0.40              |
| 1:D:399:THR:O    | 1:D:403:MET:HG3  | 2.22                     | 0.40              |
| 1:D:564:ALA:HB1  | 1:D:569:VAL:O    | 2.21                     | 0.40              |
| 2:M:184:PHE:HB3  | 2:M:209:LEU:HD11 | 2.03                     | 0.40              |
| 2:M:571:LEU:HD23 | 2:M:571:LEU:HA   | 1.91                     | 0.40              |
| 2:O:245:ARG:O    | 2:O:245:ARG:HG3  | 2.16                     | 0.40              |
| 2:O:317:LYS:HA   | 2:O:318:LEU:HD23 | 2.03                     | 0.40              |
| 2:P:505:SER:CB   | 2:P:570:TYR:CE2  | 3.05                     | 0.40              |
| 1:C:325:ARG:HH11 | 1:C:325:ARG:HD2  | 1.67                     | 0.40              |
| 1:C:483:THR:HB   | 1:C:638:PRO:HB2  | 2.03                     | 0.40              |
| 1:D:287:LEU:HA   | 1:D:388:TYR:CZ   | 2.56                     | 0.40              |
| 2:M:342:MET:HB3  | 2:M:382:LEU:O    | 2.21                     | 0.40              |
| 2:N:521:THR:O    | 2:N:522:PRO:C    | 2.65                     | 0.40              |
| 2:N:621:MET:HB3  | 2:N:621:MET:HE3  | 1.30                     | 0.40              |
| 2:O:649:ARG:HG2  | 2:O:674:LEU:HD11 | 2.03                     | 0.40              |
| 2:P:201:GLY:HA2  | 9:P:1017:HOH:O   | 2.20                     | 0.40              |
| 2:P:266:ALA:O    | 2:P:269:ALA:HB3  | 2.21                     | 0.40              |
| 2:P:419:HIS:C    | 2:P:419:HIS:ND1  | 2.80                     | 0.40              |
| 2:P:510:GLN:HA   | 2:P:513:ALA:O    | 2.22                     | 0.40              |
| 1:C:122:HIS:CD2  | 9:C:1127:HOH:O   | 2.71                     | 0.40              |
| 1:C:515:ASN:HD22 | 1:C:515:ASN:HA   | 1.71                     | 0.40              |
| 1:C:596:VAL:HG21 | 1:C:632:PHE:CD2  | 2.56                     | 0.40              |
| 1:D:271:LEU:O    | 1:D:420:ILE:HD13 | 2.22                     | 0.40              |
| 2:M:343:GLY:C    | 2:M:345:ASN:H    | 2.29                     | 0.40              |
| 2:N:4:PHE:O      | 2:N:7:ILE:HG12   | 2.20                     | 0.40              |
| 2:O:142:ARG:O    | 2:O:143:ARG:C    | 2.65                     | 0.40              |
| 2:O:169:LEU:HD12 | 2:O:193:LEU:HG   | 2.04                     | 0.40              |
| 2:P:277:ILE:HD12 | 2:P:277:ILE:N    | 2.37                     | 0.40              |
| 2:P:399:PHE:CD1  | 2:P:399:PHE:N    | 2.88                     | 0.40              |
| 2:P:604:ILE:HG22 | 2:P:643:GLY:O    | 2.20                     | 0.40              |
| 2:P:627:THR:O    | 2:P:631:LEU:HB2  | 2.22                     | 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     | 671/674 (100%)   | 637 (95%)  | 31 (5%)   | 3 (0%)   | 30          | 49 |
| 1   | B     | 671/674 (100%)   | 638 (95%)  | 31 (5%)   | 2 (0%)   | 36          | 55 |
| 1   | C     | 671/674 (100%)   | 636 (95%)  | 33 (5%)   | 2 (0%)   | 36          | 55 |
| 1   | D     | 671/674 (100%)   | 632 (94%)  | 36 (5%)   | 3 (0%)   | 30          | 49 |
| 2   | M     | 726/729 (100%)   | 678 (93%)  | 41 (6%)   | 7 (1%)   | 12          | 24 |
| 2   | N     | 726/729 (100%)   | 692 (95%)  | 27 (4%)   | 7 (1%)   | 12          | 24 |
| 2   | O     | 725/729 (100%)   | 592 (82%)  | 104 (14%) | 29 (4%)  | 2           | 3  |
| 2   | P     | 726/729 (100%)   | 622 (86%)  | 78 (11%)  | 26 (4%)  | 2           | 3  |
| All | All   | 5587/5612 (100%) | 5127 (92%) | 381 (7%)  | 79 (1%)  | 9           | 17 |

All (79) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 316 | ILE  |
| 2   | O     | 335 | LYS  |
| 2   | O     | 348 | PRO  |
| 2   | O     | 372 | ASP  |
| 2   | O     | 408 | HIS  |
| 2   | O     | 428 | LEU  |
| 2   | O     | 458 | ALA  |
| 2   | O     | 470 | ASP  |
| 2   | O     | 581 | GLN  |
| 2   | O     | 726 | ASP  |
| 2   | P     | 423 | ARG  |
| 2   | P     | 424 | ASN  |
| 2   | P     | 427 | TRP  |
| 1   | A     | 267 | ASN  |
| 1   | A     | 415 | ASN  |
| 1   | B     | 473 | LEU  |
| 1   | C     | 416 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 473 | LEU  |
| 2   | M     | 315 | LYS  |
| 2   | N     | 290 | ASP  |
| 2   | N     | 315 | LYS  |
| 2   | N     | 316 | ILE  |
| 2   | N     | 658 | ILE  |
| 2   | O     | 319 | ASP  |
| 2   | O     | 358 | GLU  |
| 2   | O     | 373 | ILE  |
| 2   | O     | 478 | MET  |
| 2   | O     | 650 | THR  |
| 2   | O     | 657 | PHE  |
| 2   | P     | 319 | ASP  |
| 2   | P     | 338 | MET  |
| 2   | P     | 359 | SER  |
| 2   | P     | 370 | GLY  |
| 2   | P     | 380 | SER  |
| 2   | P     | 474 | VAL  |
| 2   | P     | 480 | VAL  |
| 2   | P     | 491 | ARG  |
| 2   | M     | 228 | MET  |
| 2   | M     | 316 | ILE  |
| 2   | M     | 345 | ASN  |
| 2   | M     | 596 | GLY  |
| 2   | M     | 658 | ILE  |
| 2   | N     | 228 | MET  |
| 2   | O     | 123 | PRO  |
| 2   | O     | 154 | PRO  |
| 2   | O     | 187 | ASP  |
| 2   | O     | 290 | ASP  |
| 2   | O     | 527 | LEU  |
| 2   | O     | 556 | GLU  |
| 2   | P     | 187 | ASP  |
| 2   | P     | 346 | ARG  |
| 2   | P     | 360 | GLU  |
| 2   | P     | 449 | VAL  |
| 2   | P     | 489 | ASP  |
| 1   | C     | 354 | GLN  |
| 2   | M     | 187 | ASP  |
| 2   | N     | 187 | ASP  |
| 2   | N     | 596 | GLY  |
| 2   | O     | 338 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 374 | ASP  |
| 2   | O     | 493 | ARG  |
| 2   | O     | 509 | CYS  |
| 2   | P     | 320 | LEU  |
| 2   | P     | 337 | ASP  |
| 2   | P     | 378 | GLU  |
| 2   | P     | 596 | GLY  |
| 1   | A     | 316 | CYS  |
| 1   | B     | 354 | GLN  |
| 1   | D     | 267 | ASN  |
| 1   | D     | 354 | GLN  |
| 2   | O     | 345 | ASN  |
| 2   | O     | 406 | ARG  |
| 2   | P     | 10  | GLY  |
| 2   | P     | 393 | ARG  |
| 2   | P     | 379 | GLY  |
| 2   | P     | 522 | PRO  |
| 2   | P     | 336 | GLY  |
| 2   | O     | 727 | PRO  |
| 2   | P     | 638 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |    |
|-----|-------|----------------|-----------|-----------|-------------|----|
| 1   | A     | 542/543 (100%) | 507 (94%) | 35 (6%)   | 15          | 32 |
| 1   | B     | 542/543 (100%) | 517 (95%) | 25 (5%)   | 24          | 48 |
| 1   | C     | 542/543 (100%) | 500 (92%) | 42 (8%)   | 12          | 25 |
| 1   | D     | 542/543 (100%) | 504 (93%) | 38 (7%)   | 14          | 29 |
| 2   | M     | 610/611 (100%) | 551 (90%) | 59 (10%)  | 8           | 17 |
| 2   | N     | 610/611 (100%) | 561 (92%) | 49 (8%)   | 11          | 24 |
| 2   | O     | 608/611 (100%) | 463 (76%) | 145 (24%) | 1           | 1  |
| 2   | P     | 610/611 (100%) | 513 (84%) | 97 (16%)  | 2           | 5  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers  | Percentiles        |
|-----|-------|------------------|------------|-----------|--------------------|
| All | All   | 4606/4616 (100%) | 4116 (89%) | 490 (11%) | <b>6</b> <b>14</b> |

All (490) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 15     | GLU  |
| 1   | A     | 27     | ARG  |
| 1   | A     | 118    | ASN  |
| 1   | A     | 126    | GLU  |
| 1   | A     | 145    | GLU  |
| 1   | A     | 148[A] | ARG  |
| 1   | A     | 153    | GLU  |
| 1   | A     | 168    | GLU  |
| 1   | A     | 206    | PHE  |
| 1   | A     | 293    | GLN  |
| 1   | A     | 299    | GLU  |
| 1   | A     | 318    | THR  |
| 1   | A     | 331    | VAL  |
| 1   | A     | 336    | SER  |
| 1   | A     | 339    | LEU  |
| 1   | A     | 370    | ARG  |
| 1   | A     | 395    | GLU  |
| 1   | A     | 398    | LYS  |
| 1   | A     | 405    | ILE  |
| 1   | A     | 415    | ASN  |
| 1   | A     | 416    | ARG  |
| 1   | A     | 426    | ARG  |
| 1   | A     | 438    | LYS  |
| 1   | A     | 461    | LEU  |
| 1   | A     | 466    | LEU  |
| 1   | A     | 482    | LEU  |
| 1   | A     | 501    | SER  |
| 1   | A     | 518    | THR  |
| 1   | A     | 530    | ARG  |
| 1   | A     | 538    | GLU  |
| 1   | A     | 585    | SER  |
| 1   | A     | 647    | ASP  |
| 1   | A     | 656    | LEU  |
| 1   | A     | 664    | GLU  |
| 1   | A     | 665[A] | ARG  |
| 1   | B     | 82[A]  | ASP  |
| 1   | B     | 114[A] | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 159 | VAL  |
| 1   | B     | 206 | PHE  |
| 1   | B     | 298 | MET  |
| 1   | B     | 318 | THR  |
| 1   | B     | 336 | SER  |
| 1   | B     | 394 | ILE  |
| 1   | B     | 395 | GLU  |
| 1   | B     | 406 | GLU  |
| 1   | B     | 413 | GLU  |
| 1   | B     | 415 | ASN  |
| 1   | B     | 416 | ARG  |
| 1   | B     | 418 | VAL  |
| 1   | B     | 427 | VAL  |
| 1   | B     | 447 | ASN  |
| 1   | B     | 466 | LEU  |
| 1   | B     | 470 | CYS  |
| 1   | B     | 482 | LEU  |
| 1   | B     | 518 | THR  |
| 1   | B     | 531 | LEU  |
| 1   | B     | 539 | ILE  |
| 1   | B     | 600 | VAL  |
| 1   | B     | 647 | ASP  |
| 1   | B     | 656 | LEU  |
| 1   | C     | 12  | ARG  |
| 1   | C     | 23  | LYS  |
| 1   | C     | 66  | ILE  |
| 1   | C     | 82  | ASP  |
| 1   | C     | 86  | SER  |
| 1   | C     | 114 | CYS  |
| 1   | C     | 118 | ASN  |
| 1   | C     | 159 | VAL  |
| 1   | C     | 196 | GLU  |
| 1   | C     | 206 | PHE  |
| 1   | C     | 218 | GLN  |
| 1   | C     | 233 | SER  |
| 1   | C     | 260 | GLN  |
| 1   | C     | 291 | ILE  |
| 1   | C     | 331 | VAL  |
| 1   | C     | 359 | SER  |
| 1   | C     | 360 | ILE  |
| 1   | C     | 370 | ARG  |
| 1   | C     | 384 | TYR  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | C     | 409    | LYS  |
| 1   | C     | 411    | ARG  |
| 1   | C     | 412    | LYS  |
| 1   | C     | 413    | GLU  |
| 1   | C     | 416    | ARG  |
| 1   | C     | 427    | VAL  |
| 1   | C     | 438    | LYS  |
| 1   | C     | 466    | LEU  |
| 1   | C     | 470    | CYS  |
| 1   | C     | 482    | LEU  |
| 1   | C     | 501    | SER  |
| 1   | C     | 503    | GLN  |
| 1   | C     | 507    | LYS  |
| 1   | C     | 533    | GLU  |
| 1   | C     | 539[A] | ILE  |
| 1   | C     | 579    | SER  |
| 1   | C     | 585    | SER  |
| 1   | C     | 600    | VAL  |
| 1   | C     | 647    | ASP  |
| 1   | C     | 653    | THR  |
| 1   | C     | 656    | LEU  |
| 1   | C     | 664    | GLU  |
| 1   | C     | 669    | LYS  |
| 1   | D     | 3      | ARG  |
| 1   | D     | 12     | ARG  |
| 1   | D     | 40     | SER  |
| 1   | D     | 61     | ILE  |
| 1   | D     | 66     | ILE  |
| 1   | D     | 77     | ARG  |
| 1   | D     | 82     | ASP  |
| 1   | D     | 105    | MET  |
| 1   | D     | 155    | GLU  |
| 1   | D     | 159    | VAL  |
| 1   | D     | 190    | ILE  |
| 1   | D     | 199    | ARG  |
| 1   | D     | 206    | PHE  |
| 1   | D     | 275    | GLN  |
| 1   | D     | 293    | GLN  |
| 1   | D     | 296    | ARG  |
| 1   | D     | 298    | MET  |
| 1   | D     | 299    | GLU  |
| 1   | D     | 326    | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 331 | VAL  |
| 1   | D     | 395 | GLU  |
| 1   | D     | 396 | SER  |
| 1   | D     | 409 | LYS  |
| 1   | D     | 418 | VAL  |
| 1   | D     | 427 | VAL  |
| 1   | D     | 466 | LEU  |
| 1   | D     | 470 | CYS  |
| 1   | D     | 482 | LEU  |
| 1   | D     | 496 | VAL  |
| 1   | D     | 518 | THR  |
| 1   | D     | 529 | LYS  |
| 1   | D     | 533 | GLU  |
| 1   | D     | 539 | ILE  |
| 1   | D     | 600 | VAL  |
| 1   | D     | 613 | SER  |
| 1   | D     | 647 | ASP  |
| 1   | D     | 656 | LEU  |
| 1   | D     | 664 | GLU  |
| 2   | M     | 6   | LYS  |
| 2   | M     | 16  | LYS  |
| 2   | M     | 17  | GLU  |
| 2   | M     | 19  | VAL  |
| 2   | M     | 62  | LEU  |
| 2   | M     | 64  | VAL  |
| 2   | M     | 66  | ARG  |
| 2   | M     | 95  | ASN  |
| 2   | M     | 127 | LEU  |
| 2   | M     | 152 | THR  |
| 2   | M     | 164 | LYS  |
| 2   | M     | 169 | LEU  |
| 2   | M     | 174 | LYS  |
| 2   | M     | 198 | VAL  |
| 2   | M     | 214 | GLN  |
| 2   | M     | 215 | ILE  |
| 2   | M     | 221 | TYR  |
| 2   | M     | 245 | ARG  |
| 2   | M     | 249 | ARG  |
| 2   | M     | 262 | LYS  |
| 2   | M     | 284 | GLU  |
| 2   | M     | 315 | LYS  |
| 2   | M     | 317 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 334 | ARG  |
| 2   | M     | 335 | LYS  |
| 2   | M     | 342 | MET  |
| 2   | M     | 354 | ARG  |
| 2   | M     | 373 | ILE  |
| 2   | M     | 375 | GLN  |
| 2   | M     | 381 | LYS  |
| 2   | M     | 382 | LEU  |
| 2   | M     | 422 | GLN  |
| 2   | M     | 424 | ASN  |
| 2   | M     | 425 | ILE  |
| 2   | M     | 426 | ASN  |
| 2   | M     | 442 | LYS  |
| 2   | M     | 448 | LEU  |
| 2   | M     | 470 | ASP  |
| 2   | M     | 475 | LYS  |
| 2   | M     | 478 | MET  |
| 2   | M     | 479 | GLU  |
| 2   | M     | 486 | LYS  |
| 2   | M     | 539 | SER  |
| 2   | M     | 571 | LEU  |
| 2   | M     | 602 | MET  |
| 2   | M     | 604 | ILE  |
| 2   | M     | 621 | MET  |
| 2   | M     | 631 | LEU  |
| 2   | M     | 634 | MET  |
| 2   | M     | 672 | LYS  |
| 2   | M     | 674 | LEU  |
| 2   | M     | 686 | SER  |
| 2   | M     | 693 | GLU  |
| 2   | M     | 702 | GLU  |
| 2   | M     | 704 | ILE  |
| 2   | M     | 711 | ILE  |
| 2   | M     | 723 | LEU  |
| 2   | M     | 726 | ASP  |
| 2   | M     | 729 | MET  |
| 2   | N     | 6   | LYS  |
| 2   | N     | 14  | GLU  |
| 2   | N     | 64  | VAL  |
| 2   | N     | 66  | ARG  |
| 2   | N     | 95  | ASN  |
| 2   | N     | 122 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 147 | LYS  |
| 2   | N     | 152 | THR  |
| 2   | N     | 167 | LYS  |
| 2   | N     | 174 | LYS  |
| 2   | N     | 198 | VAL  |
| 2   | N     | 205 | ILE  |
| 2   | N     | 249 | ARG  |
| 2   | N     | 262 | LYS  |
| 2   | N     | 313 | LEU  |
| 2   | N     | 314 | THR  |
| 2   | N     | 316 | ILE  |
| 2   | N     | 334 | ARG  |
| 2   | N     | 335 | LYS  |
| 2   | N     | 354 | ARG  |
| 2   | N     | 362 | THR  |
| 2   | N     | 373 | ILE  |
| 2   | N     | 381 | LYS  |
| 2   | N     | 396 | GLN  |
| 2   | N     | 405 | ARG  |
| 2   | N     | 424 | ASN  |
| 2   | N     | 425 | ILE  |
| 2   | N     | 437 | LYS  |
| 2   | N     | 440 | ARG  |
| 2   | N     | 442 | LYS  |
| 2   | N     | 448 | LEU  |
| 2   | N     | 451 | LYS  |
| 2   | N     | 462 | ARG  |
| 2   | N     | 470 | ASP  |
| 2   | N     | 475 | LYS  |
| 2   | N     | 478 | MET  |
| 2   | N     | 495 | LEU  |
| 2   | N     | 571 | LEU  |
| 2   | N     | 588 | MET  |
| 2   | N     | 604 | ILE  |
| 2   | N     | 606 | PRO  |
| 2   | N     | 631 | LEU  |
| 2   | N     | 639 | THR  |
| 2   | N     | 674 | LEU  |
| 2   | N     | 675 | LYS  |
| 2   | N     | 686 | SER  |
| 2   | N     | 693 | GLU  |
| 2   | N     | 704 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 729 | MET  |
| 2   | O     | 2   | THR  |
| 2   | O     | 3   | ASP  |
| 2   | O     | 5   | ASP  |
| 2   | O     | 7   | ILE  |
| 2   | O     | 14  | GLU  |
| 2   | O     | 16  | LYS  |
| 2   | O     | 17  | GLU  |
| 2   | O     | 19  | VAL  |
| 2   | O     | 34  | SER  |
| 2   | O     | 39  | LEU  |
| 2   | O     | 62  | LEU  |
| 2   | O     | 64  | VAL  |
| 2   | O     | 66  | ARG  |
| 2   | O     | 86  | LYS  |
| 2   | O     | 95  | ASN  |
| 2   | O     | 97  | GLU  |
| 2   | O     | 122 | LYS  |
| 2   | O     | 125 | GLU  |
| 2   | O     | 127 | LEU  |
| 2   | O     | 164 | LYS  |
| 2   | O     | 174 | LYS  |
| 2   | O     | 198 | VAL  |
| 2   | O     | 205 | ILE  |
| 2   | O     | 224 | ARG  |
| 2   | O     | 228 | MET  |
| 2   | O     | 245 | ARG  |
| 2   | O     | 262 | LYS  |
| 2   | O     | 284 | GLU  |
| 2   | O     | 285 | ASP  |
| 2   | O     | 286 | LYS  |
| 2   | O     | 303 | GLN  |
| 2   | O     | 307 | GLU  |
| 2   | O     | 313 | LEU  |
| 2   | O     | 314 | THR  |
| 2   | O     | 318 | LEU  |
| 2   | O     | 320 | LEU  |
| 2   | O     | 323 | ASN  |
| 2   | O     | 332 | SER  |
| 2   | O     | 334 | ARG  |
| 2   | O     | 335 | LYS  |
| 2   | O     | 340 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 342 | MET  |
| 2   | O     | 346 | ARG  |
| 2   | O     | 347 | THR  |
| 2   | O     | 350 | PHE  |
| 2   | O     | 352 | LEU  |
| 2   | O     | 354 | ARG  |
| 2   | O     | 356 | VAL  |
| 2   | O     | 357 | SER  |
| 2   | O     | 358 | GLU  |
| 2   | O     | 359 | SER  |
| 2   | O     | 361 | ILE  |
| 2   | O     | 362 | THR  |
| 2   | O     | 366 | ILE  |
| 2   | O     | 367 | GLU  |
| 2   | O     | 368 | VAL  |
| 2   | O     | 373 | ILE  |
| 2   | O     | 375 | GLN  |
| 2   | O     | 376 | ILE  |
| 2   | O     | 378 | GLU  |
| 2   | O     | 384 | LEU  |
| 2   | O     | 386 | ILE  |
| 2   | O     | 388 | VAL  |
| 2   | O     | 393 | ARG  |
| 2   | O     | 394 | LYS  |
| 2   | O     | 399 | PHE  |
| 2   | O     | 402 | VAL  |
| 2   | O     | 403 | LEU  |
| 2   | O     | 405 | ARG  |
| 2   | O     | 406 | ARG  |
| 2   | O     | 409 | ASP  |
| 2   | O     | 420 | THR  |
| 2   | O     | 425 | ILE  |
| 2   | O     | 426 | ASN  |
| 2   | O     | 427 | TRP  |
| 2   | O     | 428 | LEU  |
| 2   | O     | 429 | ARG  |
| 2   | O     | 432 | LYS  |
| 2   | O     | 451 | LYS  |
| 2   | O     | 461 | ASP  |
| 2   | O     | 463 | VAL  |
| 2   | O     | 465 | VAL  |
| 2   | O     | 466 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 469 | THR  |
| 2   | O     | 473 | LYS  |
| 2   | O     | 474 | VAL  |
| 2   | O     | 476 | GLU  |
| 2   | O     | 478 | MET  |
| 2   | O     | 482 | ARG  |
| 2   | O     | 485 | TYR  |
| 2   | O     | 486 | LYS  |
| 2   | O     | 487 | GLU  |
| 2   | O     | 488 | ARG  |
| 2   | O     | 489 | ASP  |
| 2   | O     | 490 | ASP  |
| 2   | O     | 491 | ARG  |
| 2   | O     | 492 | MET  |
| 2   | O     | 493 | ARG  |
| 2   | O     | 495 | LEU  |
| 2   | O     | 496 | THR  |
| 2   | O     | 497 | ASP  |
| 2   | O     | 523 | GLU  |
| 2   | O     | 524 | ARG  |
| 2   | O     | 525 | VAL  |
| 2   | O     | 527 | LEU  |
| 2   | O     | 534 | LEU  |
| 2   | O     | 544 | HIS  |
| 2   | O     | 560 | ILE  |
| 2   | O     | 565 | LYS  |
| 2   | O     | 567 | VAL  |
| 2   | O     | 575 | SER  |
| 2   | O     | 577 | ARG  |
| 2   | O     | 579 | LEU  |
| 2   | O     | 582 | VAL  |
| 2   | O     | 586 | THR  |
| 2   | O     | 594 | SER  |
| 2   | O     | 598 | PHE  |
| 2   | O     | 604 | ILE  |
| 2   | O     | 609 | ASN  |
| 2   | O     | 612 | MET  |
| 2   | O     | 614 | THR  |
| 2   | O     | 615 | THR  |
| 2   | O     | 621 | MET  |
| 2   | O     | 631 | LEU  |
| 2   | O     | 634 | MET  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | O     | 635    | ILE  |
| 2   | O     | 639    | THR  |
| 2   | O     | 640    | GLN  |
| 2   | O     | 641    | THR  |
| 2   | O     | 658    | ILE  |
| 2   | O     | 664    | ILE  |
| 2   | O     | 670    | MET  |
| 2   | O     | 672    | LYS  |
| 2   | O     | 675    | LYS  |
| 2   | O     | 681    | GLU  |
| 2   | O     | 683    | VAL  |
| 2   | O     | 687    | VAL  |
| 2   | O     | 689    | GLU  |
| 2   | O     | 693    | GLU  |
| 2   | O     | 704    | ILE  |
| 2   | O     | 708    | VAL  |
| 2   | O     | 710    | GLU  |
| 2   | O     | 712    | LEU  |
| 2   | O     | 725    | MET  |
| 2   | O     | 728    | ILE  |
| 2   | P     | 6      | LYS  |
| 2   | P     | 9      | GLU  |
| 2   | P     | 39     | LEU  |
| 2   | P     | 64     | VAL  |
| 2   | P     | 66     | ARG  |
| 2   | P     | 95     | ASN  |
| 2   | P     | 125    | GLU  |
| 2   | P     | 130    | PRO  |
| 2   | P     | 146[A] | ILE  |
| 2   | P     | 152    | THR  |
| 2   | P     | 171    | LYS  |
| 2   | P     | 174    | LYS  |
| 2   | P     | 182    | MET  |
| 2   | P     | 183    | LEU  |
| 2   | P     | 198    | VAL  |
| 2   | P     | 199    | LYS  |
| 2   | P     | 205    | ILE  |
| 2   | P     | 245    | ARG  |
| 2   | P     | 262    | LYS  |
| 2   | P     | 284    | GLU  |
| 2   | P     | 286    | LYS  |
| 2   | P     | 312    | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 313 | LEU  |
| 2   | P     | 314 | THR  |
| 2   | P     | 316 | ILE  |
| 2   | P     | 318 | LEU  |
| 2   | P     | 331 | GLU  |
| 2   | P     | 334 | ARG  |
| 2   | P     | 335 | LYS  |
| 2   | P     | 340 | VAL  |
| 2   | P     | 342 | MET  |
| 2   | P     | 346 | ARG  |
| 2   | P     | 347 | THR  |
| 2   | P     | 351 | GLU  |
| 2   | P     | 353 | VAL  |
| 2   | P     | 354 | ARG  |
| 2   | P     | 355 | THR  |
| 2   | P     | 362 | THR  |
| 2   | P     | 365 | LYS  |
| 2   | P     | 366 | ILE  |
| 2   | P     | 369 | ILE  |
| 2   | P     | 373 | ILE  |
| 2   | P     | 382 | LEU  |
| 2   | P     | 388 | VAL  |
| 2   | P     | 390 | ILE  |
| 2   | P     | 393 | ARG  |
| 2   | P     | 398 | ASP  |
| 2   | P     | 403 | LEU  |
| 2   | P     | 422 | GLN  |
| 2   | P     | 424 | ASN  |
| 2   | P     | 428 | LEU  |
| 2   | P     | 431 | SER  |
| 2   | P     | 435 | VAL  |
| 2   | P     | 442 | LYS  |
| 2   | P     | 448 | LEU  |
| 2   | P     | 462 | ARG  |
| 2   | P     | 463 | VAL  |
| 2   | P     | 464 | GLN  |
| 2   | P     | 469 | THR  |
| 2   | P     | 473 | LYS  |
| 2   | P     | 474 | VAL  |
| 2   | P     | 485 | TYR  |
| 2   | P     | 486 | LYS  |
| 2   | P     | 487 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 490 | ASP  |
| 2   | P     | 495 | LEU  |
| 2   | P     | 501 | ASP  |
| 2   | P     | 527 | LEU  |
| 2   | P     | 537 | LYS  |
| 2   | P     | 541 | GLU  |
| 2   | P     | 542 | ILE  |
| 2   | P     | 551 | ILE  |
| 2   | P     | 556 | GLU  |
| 2   | P     | 563 | ILE  |
| 2   | P     | 565 | LYS  |
| 2   | P     | 567 | VAL  |
| 2   | P     | 569 | ASP  |
| 2   | P     | 571 | LEU  |
| 2   | P     | 579 | LEU  |
| 2   | P     | 605 | LEU  |
| 2   | P     | 631 | LEU  |
| 2   | P     | 639 | THR  |
| 2   | P     | 652 | ILE  |
| 2   | P     | 656 | LYS  |
| 2   | P     | 661 | ASP  |
| 2   | P     | 672 | LYS  |
| 2   | P     | 674 | LEU  |
| 2   | P     | 678 | LEU  |
| 2   | P     | 681 | GLU  |
| 2   | P     | 685 | ARG  |
| 2   | P     | 704 | ILE  |
| 2   | P     | 707 | THR  |
| 2   | P     | 717 | GLU  |
| 2   | P     | 718 | LYS  |
| 2   | P     | 726 | ASP  |
| 2   | P     | 728 | ILE  |
| 2   | P     | 729 | MET  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 58  | GLN  |
| 1   | A     | 118 | ASN  |
| 1   | A     | 209 | HIS  |
| 1   | A     | 217 | ASN  |
| 1   | A     | 218 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 220 | HIS  |
| 1   | A     | 260 | GLN  |
| 1   | A     | 275 | GLN  |
| 1   | A     | 471 | ASN  |
| 1   | A     | 477 | GLN  |
| 1   | A     | 479 | ASN  |
| 1   | A     | 515 | ASN  |
| 1   | A     | 565 | ASN  |
| 1   | A     | 622 | GLN  |
| 1   | A     | 672 | GLN  |
| 1   | B     | 58  | GLN  |
| 1   | B     | 119 | HIS  |
| 1   | B     | 122 | HIS  |
| 1   | B     | 209 | HIS  |
| 1   | B     | 217 | ASN  |
| 1   | B     | 218 | GLN  |
| 1   | B     | 220 | HIS  |
| 1   | B     | 293 | GLN  |
| 1   | B     | 415 | ASN  |
| 1   | B     | 447 | ASN  |
| 1   | B     | 454 | GLN  |
| 1   | B     | 471 | ASN  |
| 1   | B     | 477 | GLN  |
| 1   | B     | 479 | ASN  |
| 1   | B     | 503 | GLN  |
| 1   | B     | 515 | ASN  |
| 1   | B     | 565 | ASN  |
| 1   | B     | 622 | GLN  |
| 1   | B     | 672 | GLN  |
| 1   | C     | 56  | GLN  |
| 1   | C     | 58  | GLN  |
| 1   | C     | 209 | HIS  |
| 1   | C     | 217 | ASN  |
| 1   | C     | 218 | GLN  |
| 1   | C     | 443 | GLN  |
| 1   | C     | 454 | GLN  |
| 1   | C     | 471 | ASN  |
| 1   | C     | 477 | GLN  |
| 1   | C     | 479 | ASN  |
| 1   | C     | 503 | GLN  |
| 1   | C     | 515 | ASN  |
| 1   | C     | 639 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 672 | GLN  |
| 1   | D     | 56  | GLN  |
| 1   | D     | 58  | GLN  |
| 1   | D     | 118 | ASN  |
| 1   | D     | 164 | GLN  |
| 1   | D     | 209 | HIS  |
| 1   | D     | 217 | ASN  |
| 1   | D     | 218 | GLN  |
| 1   | D     | 220 | HIS  |
| 1   | D     | 446 | GLN  |
| 1   | D     | 471 | ASN  |
| 1   | D     | 477 | GLN  |
| 1   | D     | 503 | GLN  |
| 1   | D     | 515 | ASN  |
| 1   | D     | 639 | GLN  |
| 2   | M     | 95  | ASN  |
| 2   | M     | 192 | GLN  |
| 2   | M     | 197 | ASN  |
| 2   | M     | 211 | ASN  |
| 2   | M     | 287 | GLN  |
| 2   | M     | 408 | HIS  |
| 2   | M     | 424 | ASN  |
| 2   | M     | 426 | ASN  |
| 2   | M     | 510 | GLN  |
| 2   | M     | 581 | GLN  |
| 2   | M     | 590 | ASN  |
| 2   | N     | 95  | ASN  |
| 2   | N     | 192 | GLN  |
| 2   | N     | 211 | ASN  |
| 2   | N     | 408 | HIS  |
| 2   | N     | 424 | ASN  |
| 2   | N     | 510 | GLN  |
| 2   | N     | 515 | ASN  |
| 2   | N     | 549 | GLN  |
| 2   | N     | 576 | ASN  |
| 2   | N     | 581 | GLN  |
| 2   | N     | 590 | ASN  |
| 2   | N     | 679 | HIS  |
| 2   | O     | 51  | HIS  |
| 2   | O     | 95  | ASN  |
| 2   | O     | 211 | ASN  |
| 2   | O     | 244 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 258 | HIS  |
| 2   | O     | 323 | ASN  |
| 2   | O     | 396 | GLN  |
| 2   | O     | 515 | ASN  |
| 2   | O     | 516 | HIS  |
| 2   | O     | 568 | ASN  |
| 2   | O     | 578 | ASN  |
| 2   | O     | 590 | ASN  |
| 2   | O     | 618 | HIS  |
| 2   | O     | 640 | GLN  |
| 2   | O     | 679 | HIS  |
| 2   | P     | 27  | HIS  |
| 2   | P     | 95  | ASN  |
| 2   | P     | 192 | GLN  |
| 2   | P     | 211 | ASN  |
| 2   | P     | 303 | GLN  |
| 2   | P     | 396 | GLN  |
| 2   | P     | 424 | ASN  |
| 2   | P     | 426 | ASN  |
| 2   | P     | 510 | GLN  |
| 2   | P     | 515 | ASN  |
| 2   | P     | 544 | HIS  |
| 2   | P     | 548 | ASN  |
| 2   | P     | 549 | GLN  |
| 2   | P     | 568 | ASN  |
| 2   | P     | 576 | ASN  |
| 2   | P     | 618 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 75 ligands modelled in this entry, 50 are monoatomic - leaving 25 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 | $\# Z  > 2$ |
| 3   | SF4  | N     | 900 | 2    | 0,12,12      | -    | -           | -           |      |             |
| 4   | XCC  | B     | 800 | 1    | 0,11,11      | -    | -           | -           |      |             |
| 6   | GOL  | C     | 861 | -    | 5,5,5        | 0.62 | 0           | 5,5,5       | 0.81 | 0           |
| 6   | GOL  | A     | 863 | -    | 5,5,5        | 0.63 | 0           | 5,5,5       | 2.11 | 2 (40%)     |
| 6   | GOL  | A     | 861 | -    | 5,5,5        | 0.74 | 0           | 5,5,5       | 1.36 | 1 (20%)     |
| 3   | SF4  | P     | 900 | 2    | 0,12,12      | -    | -           | -           |      |             |
| 3   | SF4  | A     | 750 | 1    | 0,12,12      | -    | -           | -           |      |             |
| 6   | GOL  | C     | 860 | -    | 5,5,5        | 0.53 | 0           | 5,5,5       | 0.70 | 0           |
| 3   | SF4  | C     | 700 | 1    | 0,12,12      | -    | -           | -           |      |             |
| 6   | GOL  | D     | 863 | -    | 5,5,5        | 0.88 | 0           | 5,5,5       | 1.42 | 1 (20%)     |
| 4   | XCC  | C     | 800 | 1    | 0,11,11      | -    | -           | -           |      |             |
| 6   | GOL  | D     | 860 | -    | 5,5,5        | 0.54 | 0           | 5,5,5       | 0.38 | 0           |
| 3   | SF4  | B     | 700 | 1    | 0,12,12      | -    | -           | -           |      |             |
| 3   | SF4  | A     | 700 | 1    | 0,12,12      | -    | -           | -           |      |             |
| 3   | SF4  | O     | 900 | 2    | 0,12,12      | -    | -           | -           |      |             |
| 6   | GOL  | A     | 862 | -    | 5,5,5        | 1.04 | 0           | 5,5,5       | 1.16 | 0           |
| 4   | XCC  | A     | 800 | 1    | 0,11,11      | -    | -           | -           |      |             |
| 6   | GOL  | B     | 860 | -    | 5,5,5        | 0.84 | 0           | 5,5,5       | 1.24 | 1 (20%)     |
| 3   | SF4  | M     | 900 | 2    | 0,12,12      | -    | -           | -           |      |             |
| 6   | GOL  | A     | 860 | -    | 5,5,5        | 1.01 | 0           | 5,5,5       | 1.78 | 2 (40%)     |
| 3   | SF4  | D     | 700 | 1    | 0,12,12      | -    | -           | -           |      |             |
| 6   | GOL  | B     | 863 | -    | 5,5,5        | 0.79 | 0           | 5,5,5       | 1.75 | 2 (40%)     |
| 6   | GOL  | B     | 861 | -    | 5,5,5        | 0.73 | 0           | 5,5,5       | 1.00 | 0           |
| 3   | SF4  | C     | 750 | 1    | 0,12,12      | -    | -           | -           |      |             |
| 4   | XCC  | D     | 800 | 1    | 0,11,11      | -    | -           | -           |      |             |

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   |
|-----|------|-------|-----|------|---------|----------|---------|
| 3   | SF4  | N     | 900 | 2    | -       | -        | 0/6/5/5 |
| 4   | XCC  | B     | 800 | 1    | -       | -        | 0/3/3/3 |
| 6   | GOL  | A     | 863 | -    | -       | 0/4/4/4  | -       |
| 6   | GOL  | A     | 861 | -    | -       | 2/4/4/4  | -       |
| 3   | SF4  | P     | 900 | 2    | -       | -        | 0/6/5/5 |
| 3   | SF4  | A     | 750 | 1    | -       | -        | 0/6/5/5 |
| 6   | GOL  | C     | 860 | -    | -       | 2/4/4/4  | -       |
| 3   | SF4  | C     | 700 | 1    | -       | -        | 0/6/5/5 |
| 6   | GOL  | D     | 863 | -    | -       | 4/4/4/4  | -       |
| 6   | GOL  | D     | 860 | -    | -       | 2/4/4/4  | -       |
| 4   | XCC  | C     | 800 | 1    | -       | -        | 0/3/3/3 |
| 4   | XCC  | D     | 800 | 1    | -       | -        | 0/3/3/3 |
| 3   | SF4  | B     | 700 | 1    | -       | -        | 0/6/5/5 |
| 3   | SF4  | A     | 700 | 1    | -       | -        | 0/6/5/5 |
| 3   | SF4  | O     | 900 | 2    | -       | -        | 0/6/5/5 |
| 6   | GOL  | A     | 862 | -    | -       | 4/4/4/4  | -       |
| 4   | XCC  | A     | 800 | 1    | -       | -        | 0/3/3/3 |
| 6   | GOL  | B     | 860 | -    | -       | 4/4/4/4  | -       |
| 3   | SF4  | M     | 900 | 2    | -       | -        | 0/6/5/5 |
| 6   | GOL  | A     | 860 | -    | -       | 2/4/4/4  | -       |
| 6   | GOL  | B     | 863 | -    | -       | 0/4/4/4  | -       |
| 3   | SF4  | D     | 700 | 1    | -       | -        | 0/6/5/5 |
| 6   | GOL  | B     | 861 | -    | -       | 4/4/4/4  | -       |
| 3   | SF4  | C     | 750 | 1    | -       | -        | 0/6/5/5 |
| 6   | GOL  | C     | 861 | -    | -       | 2/4/4/4  | -       |

There are no bond length outliers.

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 6   | A     | 863 | GOL  | O3-C3-C2 | -3.96 | 92.56       | 110.38   |
| 6   | A     | 860 | GOL  | O1-C1-C2 | 2.98  | 123.80      | 110.38   |
| 6   | B     | 863 | GOL  | O2-C2-C1 | -2.85 | 97.36       | 109.18   |
| 6   | D     | 863 | GOL  | O2-C2-C3 | 2.84  | 120.95      | 109.18   |
| 6   | A     | 861 | GOL  | O3-C3-C2 | 2.68  | 122.46      | 110.38   |
| 6   | B     | 863 | GOL  | O1-C1-C2 | -2.50 | 99.13       | 110.38   |
| 6   | A     | 863 | GOL  | C3-C2-C1 | 2.25  | 120.06      | 111.80   |
| 6   | A     | 860 | GOL  | O2-C2-C3 | -2.07 | 100.61      | 109.18   |
| 6   | B     | 860 | GOL  | O2-C2-C3 | -2.02 | 100.82      | 109.18   |

There are no chirality outliers.

All (26) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 6   | A     | 861 | GOL  | C1-C2-C3-O3 |
| 6   | A     | 861 | GOL  | O2-C2-C3-O3 |
| 6   | A     | 862 | GOL  | O1-C1-C2-O2 |
| 6   | A     | 862 | GOL  | O1-C1-C2-C3 |
| 6   | A     | 862 | GOL  | C1-C2-C3-O3 |
| 6   | B     | 860 | GOL  | O1-C1-C2-C3 |
| 6   | B     | 860 | GOL  | C1-C2-C3-O3 |
| 6   | B     | 861 | GOL  | O1-C1-C2-C3 |
| 6   | B     | 861 | GOL  | C1-C2-C3-O3 |
| 6   | C     | 861 | GOL  | C1-C2-C3-O3 |
| 6   | D     | 860 | GOL  | C1-C2-C3-O3 |
| 6   | D     | 863 | GOL  | O1-C1-C2-C3 |
| 6   | D     | 863 | GOL  | C1-C2-C3-O3 |
| 6   | D     | 863 | GOL  | O2-C2-C3-O3 |
| 6   | C     | 860 | GOL  | O2-C2-C3-O3 |
| 6   | D     | 860 | GOL  | O2-C2-C3-O3 |
| 6   | A     | 860 | GOL  | C1-C2-C3-O3 |
| 6   | C     | 860 | GOL  | C1-C2-C3-O3 |
| 6   | A     | 860 | GOL  | O2-C2-C3-O3 |
| 6   | A     | 862 | GOL  | O2-C2-C3-O3 |
| 6   | B     | 860 | GOL  | O2-C2-C3-O3 |
| 6   | B     | 861 | GOL  | O1-C1-C2-O2 |
| 6   | B     | 861 | GOL  | O2-C2-C3-O3 |
| 6   | C     | 861 | GOL  | O2-C2-C3-O3 |
| 6   | B     | 860 | GOL  | O1-C1-C2-O2 |
| 6   | D     | 863 | GOL  | O1-C1-C2-O2 |

There are no ring outliers.

14 monomers are involved in 34 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | B     | 800 | XCC  | 3       | 0            |
| 6   | C     | 861 | GOL  | 1       | 0            |
| 6   | A     | 861 | GOL  | 1       | 0            |
| 3   | P     | 900 | SF4  | 1       | 0            |
| 6   | D     | 863 | GOL  | 6       | 0            |
| 4   | C     | 800 | XCC  | 3       | 0            |
| 6   | D     | 860 | GOL  | 1       | 0            |
| 3   | B     | 700 | SF4  | 1       | 0            |
| 3   | O     | 900 | SF4  | 5       | 0            |
| 6   | A     | 862 | GOL  | 4       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | A     | 800 | XCC  | 2       | 0            |
| 6   | B     | 863 | GOL  | 2       | 0            |
| 6   | B     | 861 | GOL  | 3       | 0            |
| 4   | D     | 800 | XCC  | 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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2                                  | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|------------------------------------------|-----------------------|---------|
| 1   | A     | 673/674 (99%)   | -0.73  | 0 <span>100</span> <span>100</span>      | 9, 18, 36, 61         | 2 (0%)  |
| 1   | B     | 673/674 (99%)   | -0.77  | 1 (0%) <span>92</span> <span>90</span>   | 8, 18, 35, 67         | 7 (1%)  |
| 1   | C     | 673/674 (99%)   | -0.54  | 2 (0%) <span>90</span> <span>87</span>   | 10, 23, 40, 61        | 3 (0%)  |
| 1   | D     | 673/674 (99%)   | -0.45  | 2 (0%) <span>90</span> <span>87</span>   | 11, 25, 46, 70        | 2 (0%)  |
| 2   | M     | 728/729 (99%)   | -0.45  | 4 (0%) <span>87</span> <span>85</span>   | 9, 25, 49, 70         | 4 (0%)  |
| 2   | N     | 728/729 (99%)   | -0.54  | 3 (0%) <span>88</span> <span>86</span>   | 7, 23, 48, 64         | 3 (0%)  |
| 2   | O     | 727/729 (99%)   | 1.17   | 178 (24%) <span>2</span> <span>1</span>  | 22, 58, 90, 130       | 1 (0%)  |
| 2   | P     | 728/729 (99%)   | 0.40   | 90 (12%) <span>8</span> <span>6</span>   | 12, 40, 84, 112       | 3 (0%)  |
| All | All   | 5603/5612 (99%) | -0.22  | 280 (4%) <span>34</span> <span>30</span> | 7, 25, 71, 130        | 25 (0%) |

All (280) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | O     | 728 | ILE  | 6.0  |
| 2   | O     | 480 | VAL  | 5.4  |
| 2   | O     | 356 | VAL  | 5.3  |
| 2   | P     | 480 | VAL  | 4.9  |
| 2   | P     | 356 | VAL  | 4.7  |
| 2   | O     | 350 | PHE  | 4.7  |
| 2   | O     | 723 | LEU  | 4.6  |
| 2   | O     | 399 | PHE  | 4.6  |
| 2   | O     | 465 | VAL  | 4.3  |
| 2   | P     | 387 | LEU  | 4.3  |
| 1   | B     | 539 | ILE  | 4.3  |
| 2   | P     | 485 | TYR  | 4.3  |
| 2   | P     | 335 | LYS  | 4.2  |
| 2   | O     | 485 | TYR  | 4.2  |
| 2   | O     | 384 | LEU  | 4.2  |
| 2   | P     | 346 | ARG  | 4.2  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | C     | 539[A] | ILE  | 4.1  |
| 2   | O     | 382    | LEU  | 4.1  |
| 2   | O     | 402    | VAL  | 4.0  |
| 2   | P     | 355    | THR  | 3.9  |
| 2   | P     | 399    | PHE  | 3.8  |
| 2   | O     | 353    | VAL  | 3.8  |
| 2   | P     | 474    | VAL  | 3.8  |
| 2   | P     | 352    | LEU  | 3.8  |
| 2   | O     | 469    | THR  | 3.8  |
| 2   | P     | 343    | GLY  | 3.8  |
| 2   | P     | 459    | ILE  | 3.8  |
| 2   | O     | 474    | VAL  | 3.7  |
| 2   | P     | 353    | VAL  | 3.7  |
| 2   | O     | 457    | PRO  | 3.7  |
| 2   | O     | 486    | LYS  | 3.7  |
| 2   | M     | 314    | THR  | 3.7  |
| 2   | O     | 488    | ARG  | 3.7  |
| 2   | M     | 729    | MET  | 3.6  |
| 2   | P     | 391    | TYR  | 3.6  |
| 2   | P     | 475    | LYS  | 3.6  |
| 2   | O     | 318    | LEU  | 3.6  |
| 2   | P     | 481    | ALA  | 3.5  |
| 2   | O     | 459    | ILE  | 3.5  |
| 2   | O     | 579    | LEU  | 3.5  |
| 2   | O     | 472    | ALA  | 3.5  |
| 2   | P     | 425    | ILE  | 3.5  |
| 2   | O     | 460    | VAL  | 3.4  |
| 2   | P     | 384    | LEU  | 3.4  |
| 2   | O     | 377    | PRO  | 3.4  |
| 2   | P     | 458    | ALA  | 3.4  |
| 2   | O     | 369    | ILE  | 3.4  |
| 2   | P     | 316    | ILE  | 3.4  |
| 2   | O     | 492    | MET  | 3.4  |
| 2   | P     | 486    | LYS  | 3.4  |
| 2   | O     | 463    | VAL  | 3.4  |
| 2   | P     | 463    | VAL  | 3.4  |
| 1   | D     | 539    | ILE  | 3.4  |
| 2   | O     | 519    | ILE  | 3.3  |
| 2   | P     | 484    | LYS  | 3.3  |
| 2   | O     | 520    | VAL  | 3.3  |
| 2   | P     | 457    | PRO  | 3.3  |
| 2   | O     | 340    | VAL  | 3.3  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 2   | O     | 692    | GLY  | 3.3  |
| 2   | O     | 725    | MET  | 3.3  |
| 2   | P     | 472    | ALA  | 3.3  |
| 2   | O     | 566    | SER  | 3.2  |
| 2   | O     | 504    | TYR  | 3.2  |
| 2   | P     | 345    | ASN  | 3.2  |
| 2   | O     | 724    | THR  | 3.2  |
| 2   | O     | 495    | LEU  | 3.2  |
| 2   | P     | 357    | SER  | 3.2  |
| 2   | O     | 314    | THR  | 3.2  |
| 2   | O     | 653    | VAL  | 3.2  |
| 2   | O     | 366    | ILE  | 3.2  |
| 2   | O     | 481    | ALA  | 3.1  |
| 2   | P     | 336    | GLY  | 3.1  |
| 2   | O     | 530    | ALA  | 3.1  |
| 2   | P     | 315[A] | LYS  | 3.1  |
| 2   | P     | 350    | PHE  | 3.1  |
| 2   | O     | 533    | TRP  | 3.1  |
| 2   | O     | 403    | LEU  | 3.1  |
| 2   | P     | 488    | ARG  | 3.1  |
| 2   | O     | 401    | GLY  | 3.1  |
| 2   | O     | 376    | ILE  | 3.1  |
| 2   | O     | 355    | THR  | 3.0  |
| 2   | P     | 342    | MET  | 3.0  |
| 2   | O     | 545    | ALA  | 3.0  |
| 2   | P     | 344    | GLY  | 3.0  |
| 2   | P     | 390    | ILE  | 3.0  |
| 2   | P     | 467    | ILE  | 3.0  |
| 2   | O     | 482    | ARG  | 3.0  |
| 2   | P     | 461    | ASP  | 3.0  |
| 2   | O     | 316    | ILE  | 3.0  |
| 2   | O     | 368    | VAL  | 3.0  |
| 2   | P     | 460    | VAL  | 3.0  |
| 2   | P     | 427    | TRP  | 3.0  |
| 2   | O     | 339    | TYR  | 3.0  |
| 2   | O     | 491    | ARG  | 3.0  |
| 2   | P     | 482    | ARG  | 3.0  |
| 2   | O     | 529    | GLY  | 3.0  |
| 2   | O     | 447    | ILE  | 2.9  |
| 2   | O     | 542    | ILE  | 2.9  |
| 2   | P     | 354    | ARG  | 2.9  |
| 2   | O     | 428    | LEU  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | O     | 359 | SER  | 2.9  |
| 2   | O     | 467 | ILE  | 2.9  |
| 2   | P     | 729 | MET  | 2.9  |
| 2   | O     | 687 | VAL  | 2.9  |
| 2   | O     | 420 | THR  | 2.9  |
| 2   | O     | 371 | PRO  | 2.9  |
| 2   | P     | 469 | THR  | 2.9  |
| 2   | P     | 724 | THR  | 2.9  |
| 2   | O     | 564 | TRP  | 2.9  |
| 2   | O     | 655 | LYS  | 2.9  |
| 2   | P     | 381 | LYS  | 2.9  |
| 2   | O     | 410 | PHE  | 2.9  |
| 2   | O     | 448 | LEU  | 2.8  |
| 2   | O     | 470 | ASP  | 2.8  |
| 2   | P     | 728 | ILE  | 2.8  |
| 2   | O     | 500 | VAL  | 2.8  |
| 2   | O     | 362 | THR  | 2.8  |
| 2   | O     | 450 | ALA  | 2.8  |
| 2   | O     | 342 | MET  | 2.8  |
| 2   | O     | 348 | PRO  | 2.8  |
| 2   | O     | 2   | THR  | 2.8  |
| 2   | O     | 567 | VAL  | 2.7  |
| 2   | P     | 314 | THR  | 2.7  |
| 2   | O     | 494 | GLY  | 2.7  |
| 2   | P     | 338 | MET  | 2.7  |
| 2   | O     | 390 | ILE  | 2.7  |
| 2   | N     | 318 | LEU  | 2.7  |
| 2   | P     | 395 | MET  | 2.7  |
| 2   | P     | 477 | TYR  | 2.7  |
| 1   | D     | 416 | ARG  | 2.7  |
| 2   | O     | 466 | THR  | 2.7  |
| 2   | O     | 373 | ILE  | 2.7  |
| 2   | O     | 468 | PHE  | 2.7  |
| 2   | O     | 380 | SER  | 2.7  |
| 2   | O     | 582 | VAL  | 2.7  |
| 2   | O     | 572 | TYR  | 2.7  |
| 2   | O     | 427 | TRP  | 2.7  |
| 2   | P     | 573 | THR  | 2.7  |
| 2   | O     | 596 | GLY  | 2.6  |
| 2   | O     | 484 | LYS  | 2.6  |
| 2   | O     | 550 | PRO  | 2.6  |
| 2   | P     | 424 | ASN  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | O     | 691 | LEU  | 2.6  |
| 2   | P     | 495 | LEU  | 2.6  |
| 2   | O     | 538 | ALA  | 2.6  |
| 2   | O     | 344 | GLY  | 2.6  |
| 2   | O     | 379 | GLY  | 2.6  |
| 2   | P     | 394 | LYS  | 2.6  |
| 2   | P     | 473 | LYS  | 2.6  |
| 2   | O     | 383 | PRO  | 2.6  |
| 2   | P     | 557 | ILE  | 2.6  |
| 2   | O     | 378 | GLU  | 2.6  |
| 2   | O     | 388 | VAL  | 2.6  |
| 2   | O     | 668 | VAL  | 2.6  |
| 2   | P     | 347 | THR  | 2.6  |
| 2   | O     | 391 | TYR  | 2.6  |
| 2   | P     | 364 | GLY  | 2.6  |
| 2   | P     | 552 | PRO  | 2.6  |
| 2   | O     | 551 | ILE  | 2.6  |
| 2   | O     | 534 | LEU  | 2.6  |
| 2   | P     | 723 | LEU  | 2.6  |
| 2   | O     | 525 | VAL  | 2.6  |
| 2   | O     | 475 | LYS  | 2.6  |
| 2   | P     | 348 | PRO  | 2.6  |
| 2   | O     | 696 | ILE  | 2.6  |
| 2   | O     | 431 | SER  | 2.6  |
| 2   | O     | 570 | TYR  | 2.6  |
| 2   | P     | 471 | GLU  | 2.5  |
| 2   | P     | 639 | THR  | 2.5  |
| 2   | O     | 338 | MET  | 2.5  |
| 2   | O     | 361 | ILE  | 2.5  |
| 2   | P     | 340 | VAL  | 2.5  |
| 1   | C     | 416 | ARG  | 2.5  |
| 2   | O     | 605 | LEU  | 2.5  |
| 2   | O     | 683 | VAL  | 2.5  |
| 2   | O     | 349 | ALA  | 2.5  |
| 2   | O     | 665 | ALA  | 2.5  |
| 2   | O     | 650 | THR  | 2.5  |
| 2   | O     | 664 | ILE  | 2.5  |
| 2   | P     | 369 | ILE  | 2.5  |
| 2   | O     | 387 | LEU  | 2.5  |
| 2   | P     | 491 | ARG  | 2.5  |
| 2   | O     | 395 | MET  | 2.5  |
| 2   | O     | 407 | ILE  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | O     | 490 | ASP  | 2.4  |
| 2   | O     | 478 | MET  | 2.4  |
| 2   | O     | 727 | PRO  | 2.4  |
| 2   | O     | 473 | LYS  | 2.4  |
| 2   | N     | 316 | ILE  | 2.4  |
| 2   | M     | 313 | LEU  | 2.4  |
| 2   | O     | 313 | LEU  | 2.4  |
| 2   | O     | 444 | TYR  | 2.4  |
| 2   | O     | 393 | ARG  | 2.4  |
| 2   | O     | 151 | TRP  | 2.4  |
| 2   | P     | 581 | GLN  | 2.4  |
| 2   | O     | 315 | LYS  | 2.4  |
| 2   | O     | 586 | THR  | 2.4  |
| 2   | O     | 385 | GLY  | 2.4  |
| 2   | O     | 456 | PHE  | 2.4  |
| 2   | O     | 540 | TYR  | 2.4  |
| 2   | P     | 478 | MET  | 2.4  |
| 2   | O     | 708 | VAL  | 2.4  |
| 2   | O     | 317 | LYS  | 2.4  |
| 2   | P     | 341 | GLU  | 2.4  |
| 2   | O     | 357 | SER  | 2.3  |
| 2   | O     | 548 | ASN  | 2.3  |
| 2   | O     | 343 | GLY  | 2.3  |
| 2   | O     | 610 | GLY  | 2.3  |
| 2   | O     | 333 | ILE  | 2.3  |
| 2   | O     | 560 | ILE  | 2.3  |
| 2   | P     | 398 | ASP  | 2.3  |
| 2   | O     | 381 | LYS  | 2.3  |
| 2   | O     | 430 | VAL  | 2.3  |
| 2   | P     | 400 | GLU  | 2.3  |
| 2   | O     | 392 | GLY  | 2.3  |
| 2   | O     | 322 | ILE  | 2.3  |
| 2   | O     | 358 | GLU  | 2.3  |
| 2   | O     | 663 | GLY  | 2.3  |
| 2   | O     | 386 | ILE  | 2.3  |
| 2   | O     | 435 | VAL  | 2.3  |
| 2   | P     | 388 | VAL  | 2.3  |
| 2   | O     | 522 | PRO  | 2.3  |
| 2   | P     | 383 | PRO  | 2.3  |
| 2   | O     | 477 | TYR  | 2.3  |
| 2   | O     | 573 | THR  | 2.2  |
| 2   | O     | 719 | GLY  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | O     | 425 | ILE  | 2.2  |
| 2   | O     | 715 | LEU  | 2.2  |
| 2   | O     | 595 | CYS  | 2.2  |
| 2   | O     | 347 | THR  | 2.2  |
| 2   | O     | 320 | LEU  | 2.2  |
| 2   | O     | 584 | LEU  | 2.2  |
| 2   | O     | 645 | MET  | 2.2  |
| 2   | O     | 489 | ASP  | 2.2  |
| 2   | O     | 406 | ARG  | 2.2  |
| 2   | O     | 453 | LYS  | 2.2  |
| 2   | P     | 719 | GLY  | 2.2  |
| 2   | P     | 359 | SER  | 2.2  |
| 2   | O     | 389 | ASP  | 2.2  |
| 2   | O     | 524 | ARG  | 2.2  |
| 2   | O     | 713 | PRO  | 2.2  |
| 2   | O     | 464 | GLN  | 2.2  |
| 2   | O     | 557 | ILE  | 2.2  |
| 2   | O     | 563 | ILE  | 2.2  |
| 2   | O     | 331 | GLU  | 2.2  |
| 2   | O     | 547 | PRO  | 2.2  |
| 2   | M     | 335 | LYS  | 2.2  |
| 2   | P     | 402 | VAL  | 2.1  |
| 2   | P     | 492 | MET  | 2.1  |
| 2   | O     | 483 | GLU  | 2.1  |
| 2   | O     | 398 | ASP  | 2.1  |
| 2   | P     | 317 | LYS  | 2.1  |
| 2   | O     | 345 | ASN  | 2.1  |
| 2   | O     | 336 | GLY  | 2.1  |
| 2   | P     | 366 | ILE  | 2.1  |
| 2   | P     | 462 | ARG  | 2.1  |
| 2   | O     | 505 | SER  | 2.1  |
| 2   | O     | 592 | MET  | 2.1  |
| 2   | P     | 493 | ARG  | 2.1  |
| 2   | P     | 542 | ILE  | 2.1  |
| 2   | P     | 570 | TYR  | 2.1  |
| 2   | O     | 553 | LYS  | 2.1  |
| 2   | P     | 623 | PRO  | 2.1  |
| 2   | O     | 439 | PHE  | 2.1  |
| 2   | O     | 458 | ALA  | 2.1  |
| 2   | P     | 349 | ALA  | 2.1  |
| 2   | N     | 335 | LYS  | 2.1  |
| 2   | O     | 612 | MET  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | O     | 544 | HIS  | 2.1  |
| 2   | O     | 695 | PHE  | 2.0  |
| 2   | O     | 397 | ALA  | 2.0  |
| 2   | P     | 397 | ALA  | 2.0  |
| 2   | P     | 650 | THR  | 2.0  |
| 2   | O     | 497 | ASP  | 2.0  |
| 2   | P     | 371 | PRO  | 2.0  |
| 2   | O     | 452 | MET  | 2.0  |
| 2   | O     | 324 | PHE  | 2.0  |
| 2   | P     | 379 | GLY  | 2.0  |
| 2   | P     | 496 | THR  | 2.0  |
| 2   | P     | 533 | TRP  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 6   | GOL  | C     | 861 | 6/6   | 0.79 | 0.14 | 53,59,59,60                | 0     |
| 6   | GOL  | D     | 860 | 6/6   | 0.84 | 0.13 | 47,51,52,52                | 0     |
| 6   | GOL  | B     | 861 | 6/6   | 0.85 | 0.16 | 45,51,52,54                | 0     |
| 6   | GOL  | C     | 860 | 6/6   | 0.85 | 0.14 | 39,48,50,51                | 0     |
| 6   | GOL  | D     | 863 | 6/6   | 0.89 | 0.14 | 28,36,42,42                | 0     |
| 6   | GOL  | B     | 863 | 6/6   | 0.91 | 0.12 | 30,34,37,37                | 0     |
| 4   | XCC  | D     | 800 | 9/9   | 0.92 | 0.09 | 52,61,69,69                | 0     |
| 6   | GOL  | A     | 861 | 6/6   | 0.92 | 0.12 | 34,47,51,53                | 0     |
| 6   | GOL  | B     | 860 | 6/6   | 0.93 | 0.09 | 27,27,30,30                | 0     |
| 6   | GOL  | A     | 863 | 6/6   | 0.94 | 0.10 | 22,26,32,35                | 0     |
| 4   | XCC  | C     | 800 | 9/9   | 0.94 | 0.08 | 40,54,66,66                | 0     |

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| Mol | Type | Chain | Res     | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|---------|-------|------|------|----------------------------|-------|
| 3   | SF4  | O     | 900     | 8/8   | 0.95 | 0.06 | 59,60,62,62                | 0     |
| 4   | XCC  | A     | 800     | 9/9   | 0.95 | 0.07 | 37,48,56,57                | 0     |
| 5   | XE   | C     | 1001    | 1/1   | 0.95 | 0.14 | 13,13,13,13                | 1     |
| 4   | XCC  | B     | 800     | 9/9   | 0.95 | 0.07 | 37,52,54,57                | 0     |
| 5   | XE   | O     | 1007    | 1/1   | 0.96 | 0.04 | 33,33,33,33                | 1     |
| 5   | XE   | P     | 1008    | 1/1   | 0.96 | 0.07 | 19,19,19,19                | 1     |
| 5   | XE   | B     | 1001    | 1/1   | 0.96 | 0.08 | 32,32,32,32                | 1     |
| 6   | GOL  | A     | 862     | 6/6   | 0.96 | 0.12 | 27,30,35,35                | 0     |
| 5   | XE   | D     | 1010    | 1/1   | 0.96 | 0.05 | 25,25,25,25                | 1     |
| 5   | XE   | M     | 1006    | 1/1   | 0.96 | 0.06 | 29,29,29,29                | 1     |
| 7   | CU1  | O     | 950     | 1/1   | 0.96 | 0.06 | 88,88,88,88                | 0     |
| 5   | XE   | O     | 1006    | 1/1   | 0.97 | 0.12 | 30,30,30,30                | 1     |
| 5   | XE   | D     | 1001    | 1/1   | 0.97 | 0.22 | 34,34,34,34                | 1     |
| 5   | XE   | N     | 1006    | 1/1   | 0.97 | 0.04 | 27,27,27,27                | 1     |
| 6   | GOL  | A     | 860     | 6/6   | 0.97 | 0.06 | 17,20,23,27                | 0     |
| 5   | XE   | N     | 1008    | 1/1   | 0.97 | 0.09 | 25,25,25,25                | 1     |
| 7   | CU1  | P     | 950     | 1/1   | 0.97 | 0.04 | 52,52,52,52                | 0     |
| 8   | NI   | O     | 951     | 1/1   | 0.97 | 0.09 | 75,75,75,75                | 0     |
| 5   | XE   | P     | 1006    | 1/1   | 0.98 | 0.07 | 29,29,29,29                | 1     |
| 7   | CU1  | M     | 950     | 1/1   | 0.98 | 0.03 | 30,30,30,30                | 0     |
| 5   | XE   | C     | 1005    | 1/1   | 0.98 | 0.02 | 31,31,31,31                | 1     |
| 5   | XE   | A     | 1001    | 1/1   | 0.98 | 0.12 | 23,23,23,23                | 1     |
| 5   | XE   | O     | 1009    | 1/1   | 0.98 | 0.05 | 42,42,42,42                | 1     |
| 3   | SF4  | B     | 700     | 8/8   | 0.99 | 0.03 | 7,9,11,15                  | 0     |
| 5   | XE   | M     | 1008    | 1/1   | 0.99 | 0.02 | 30,30,30,30                | 1     |
| 3   | SF4  | C     | 700     | 8/8   | 0.99 | 0.03 | 21,23,24,24                | 0     |
| 3   | SF4  | C     | 750     | 8/8   | 0.99 | 0.03 | 22,26,28,28                | 0     |
| 3   | SF4  | D     | 700     | 8/8   | 0.99 | 0.03 | 18,19,20,22                | 0     |
| 5   | XE   | A     | 1002    | 1/1   | 0.99 | 0.01 | 27,27,27,27                | 0     |
| 5   | XE   | A     | 1003[A] | 1/1   | 0.99 | 0.03 | 30,30,30,30                | 1     |
| 5   | XE   | A     | 1003[B] | 1/1   | 0.99 | 0.03 | 14,14,14,14                | 1     |
| 5   | XE   | P     | 1007    | 1/1   | 0.99 | 0.02 | 29,29,29,29                | 0     |
| 5   | XE   | A     | 1010    | 1/1   | 0.99 | 0.09 | 31,31,31,31                | 1     |
| 5   | XE   | P     | 1009    | 1/1   | 0.99 | 0.04 | 31,31,31,31                | 1     |
| 3   | SF4  | M     | 900     | 8/8   | 0.99 | 0.02 | 13,14,17,20                | 0     |
| 5   | XE   | B     | 1002    | 1/1   | 0.99 | 0.02 | 25,25,25,25                | 0     |
| 5   | XE   | B     | 1010    | 1/1   | 0.99 | 0.08 | 24,24,24,24                | 1     |
| 3   | SF4  | N     | 900     | 8/8   | 0.99 | 0.03 | 12,14,16,17                | 0     |
| 5   | XE   | C     | 1002    | 1/1   | 0.99 | 0.04 | 33,33,33,33                | 0     |
| 5   | XE   | C     | 1003[A] | 1/1   | 0.99 | 0.02 | 29,29,29,29                | 1     |
| 5   | XE   | C     | 1003[B] | 1/1   | 0.99 | 0.02 | 33,33,33,33                | 1     |
| 3   | SF4  | A     | 700     | 8/8   | 0.99 | 0.03 | 10,12,14,14                | 0     |

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| Mol | Type | Chain | Res     | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|---------|-------|------|------|----------------------------|-------|
| 5   | XE   | C     | 1010    | 1/1   | 0.99 | 0.04 | 35,35,35,35                | 1     |
| 3   | SF4  | P     | 900     | 8/8   | 0.99 | 0.04 | 31,34,36,37                | 0     |
| 5   | XE   | D     | 1002    | 1/1   | 0.99 | 0.03 | 29,29,29,29                | 1     |
| 5   | XE   | D     | 1003[A] | 1/1   | 0.99 | 0.04 | 28,28,28,28                | 1     |
| 7   | CU1  | N     | 950     | 1/1   | 0.99 | 0.02 | 28,28,28,28                | 0     |
| 5   | XE   | D     | 1003[B] | 1/1   | 0.99 | 0.04 | 30,30,30,30                | 1     |
| 5   | XE   | D     | 1004    | 1/1   | 0.99 | 0.02 | 28,28,28,28                | 1     |
| 3   | SF4  | A     | 750     | 8/8   | 0.99 | 0.02 | 12,15,16,17                | 0     |
| 8   | NI   | P     | 951     | 1/1   | 0.99 | 0.02 | 44,44,44,44                | 0     |
| 5   | XE   | D     | 1005    | 1/1   | 1.00 | 0.02 | 27,27,27,27                | 0     |
| 5   | XE   | B     | 1005    | 1/1   | 1.00 | 0.02 | 21,21,21,21                | 0     |
| 5   | XE   | A     | 1005    | 1/1   | 1.00 | 0.02 | 24,24,24,24                | 0     |
| 5   | XE   | M     | 1007    | 1/1   | 1.00 | 0.02 | 27,27,27,27                | 0     |
| 5   | XE   | A     | 1004    | 1/1   | 1.00 | 0.03 | 30,30,30,30                | 1     |
| 5   | XE   | B     | 1003[A] | 1/1   | 1.00 | 0.02 | 26,26,26,26                | 1     |
| 5   | XE   | N     | 1007    | 1/1   | 1.00 | 0.01 | 21,21,21,21                | 0     |
| 5   | XE   | B     | 1003[B] | 1/1   | 1.00 | 0.02 | 25,25,25,25                | 1     |
| 5   | XE   | N     | 1009    | 1/1   | 1.00 | 0.01 | 34,34,34,34                | 1     |
| 8   | NI   | M     | 951     | 1/1   | 1.00 | 0.03 | 18,18,18,18                | 0     |
| 8   | NI   | N     | 951     | 1/1   | 1.00 | 0.02 | 17,17,17,17                | 0     |
| 5   | XE   | B     | 1004    | 1/1   | 1.00 | 0.02 | 29,29,29,29                | 1     |
| 5   | XE   | C     | 1004    | 1/1   | 1.00 | 0.01 | 30,30,30,30                | 1     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.