



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:06 AM UTC

PDB ID : 3I01 / pdb\_00003i01  
Title : Native structure of bifunctional carbon monoxide dehydrogenase/acetyl-CoA synthase from Moorella thermoacetica, water-bound C-cluster.  
Authors : Kung, Y.; Doukov, T.I.; Drennan, C.L.  
Deposited on : 2009-06-24  
Resolution : 2.15 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>.

---

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                                                             |

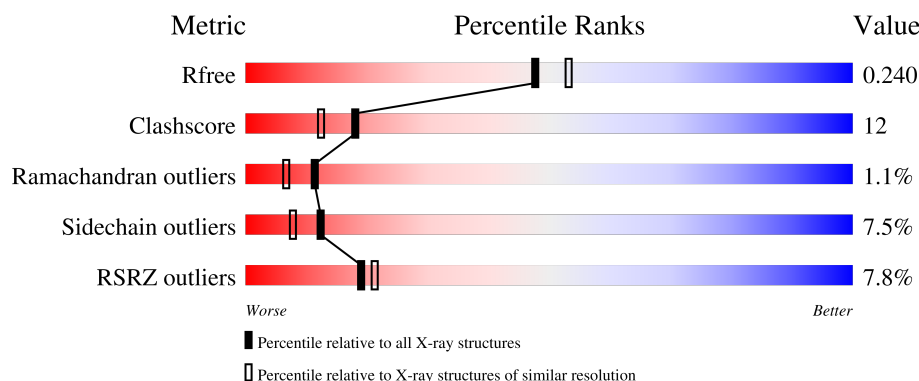
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 2057 (2.16-2.16)                                      |
| Clashscore            | 190562                      | 2159 (2.16-2.16)                                      |
| Ramachandran outliers | 187476                      | 2134 (2.16-2.16)                                      |
| Sidechain outliers    | 187428                      | 2133 (2.16-2.16)                                      |
| RSRZ outliers         | 180081                      | 2059 (2.16-2.16)                                      |

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    | <br>81% 18% .   |
| 1   | B     | 674    | <br>80% 17% .   |
| 1   | C     | 674    | <br>79% 19% .   |
| 1   | D     | 674    | <br>77% 21% .   |
| 2   | M     | 729    | <br>76% 20% . . |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | N     | 729    |                  |
| 2   | O     | 729    |                  |
| 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  | D     | 800 | -         | -        | X       | -                |
| 5   | GOL  | C     | 863 | -         | -        | X       | -                |
| 5   | GOL  | D     | 863 | -         | -        | X       | -                |

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 45096 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       | 7       | 0     |
|     |       |          | 5128  | 3223 | 897 | 966 | 42 |         |         |       |
| 1   | B     | 673      | Total | C    | N   | O   | S  | 0       | 5       | 0     |
|     |       |          | 5121  | 3221 | 895 | 963 | 42 |         |         |       |
| 1   | C     | 673      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 5094  | 3205 | 888 | 959 | 42 |         |         |       |
| 1   | D     | 673      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 5119  | 3218 | 895 | 964 | 42 |         |         |       |

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

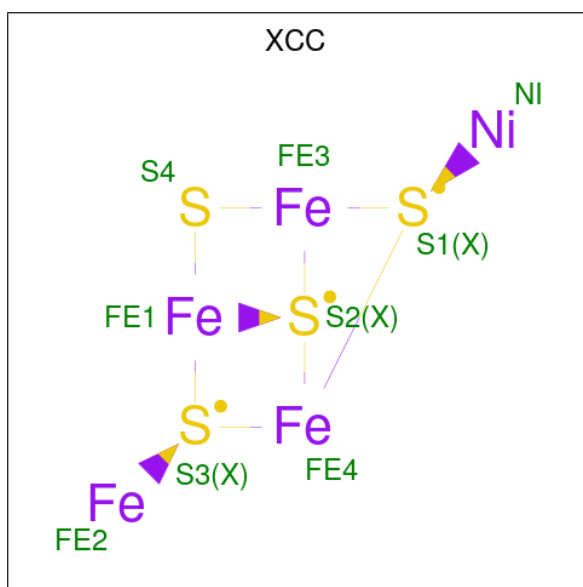
| Mol | Chain | Residues | Atoms |      |     |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|---------|-------|
| 2   | M     | 728      | Total | C    | N   | O    | S  | 0       | 5       | 0     |
|     |       |          | 5778  | 3703 | 964 | 1076 | 35 |         |         |       |
| 2   | N     | 728      | Total | C    | N   | O    | S  | 0       | 6       | 0     |
|     |       |          | 5784  | 3707 | 968 | 1074 | 35 |         |         |       |
| 2   | O     | 728      | Total | C    | N   | O    | S  | 0       | 1       | 0     |
|     |       |          | 5749  | 3687 | 958 | 1069 | 35 |         |         |       |
| 2   | P     | 728      | Total | C    | N   | O    | S  | 0       | 1       | 0     |
|     |       |          | 5746  | 3684 | 959 | 1068 | 35 |         |         |       |

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



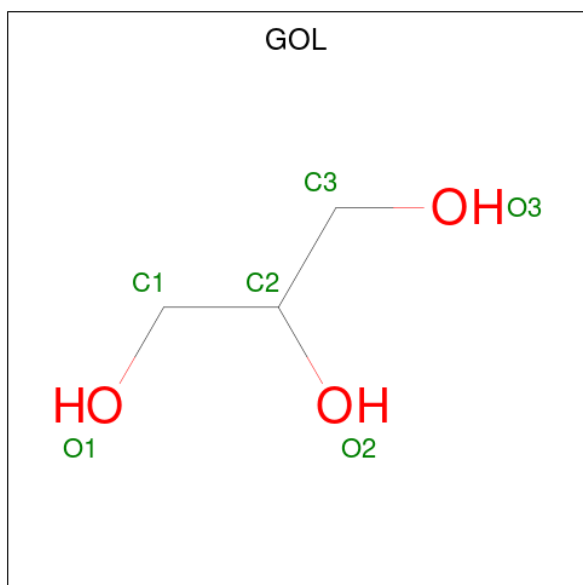
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 3   | A     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 3   | A     | 1        | Total | Fe | S | 0       | 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 GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 5   | A     | 1        | Total C O<br>6 3 3 | 0       | 0       |
| 5   | B     | 1        | Total C O<br>6 3 3 | 0       | 0       |
| 5   | C     | 1        | Total C O<br>6 3 3 | 0       | 0       |
| 5   | D     | 1        | Total C O<br>6 3 3 | 0       | 0       |

- Molecule 6 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 6   | M     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 6   | N     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 6   | O     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 6   | P     | 1        | Total Cu<br>1 1 | 0       | 0       |

- Molecule 7 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 8   | M     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 2 | 1 |         |         |
| 8   | N     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 2 | 1 |         |         |
| 8   | O     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 2 | 1 |         |         |
| 8   | P     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 2 | 1 |         |         |

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 9   | M     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 9   | N     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 9   | O     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 9   | P     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 10 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 10  | A     | 215      | Total | O   | 0       | 0       |
|     |       |          | 215   | 215 |         |         |

*Continued on next page...*

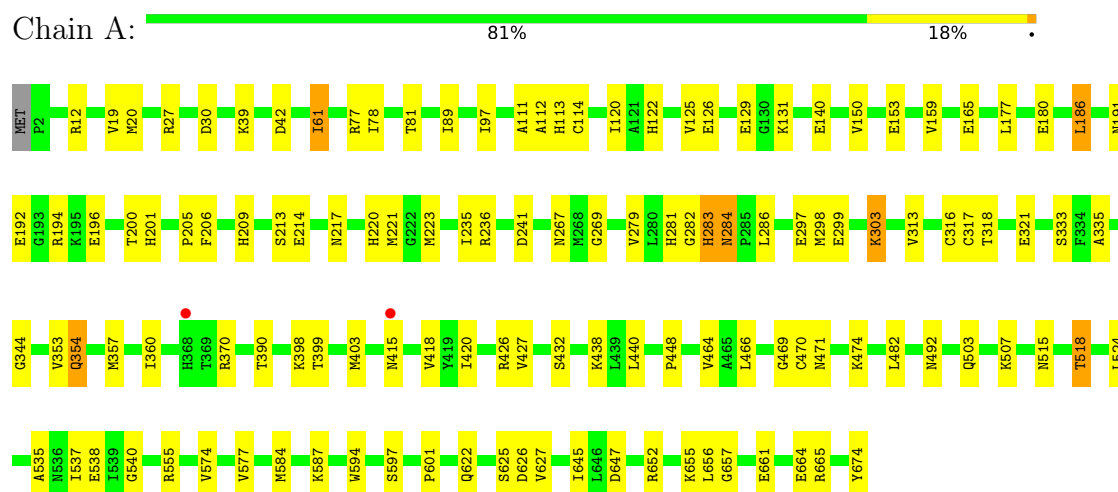
*Continued from previous page...*

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 10  | B     | 288      | Total<br>288 | O<br>288 | 0       | 0       |
| 10  | C     | 169      | Total<br>169 | O<br>169 | 0       | 0       |
| 10  | D     | 151      | Total<br>151 | O<br>151 | 0       | 0       |
| 10  | M     | 218      | Total<br>218 | O<br>218 | 0       | 0       |
| 10  | N     | 227      | Total<br>227 | O<br>227 | 0       | 0       |
| 10  | O     | 27       | Total<br>27  | O<br>27  | 0       | 0       |
| 10  | P     | 118      | Total<br>118 | O<br>118 | 0       | 0       |

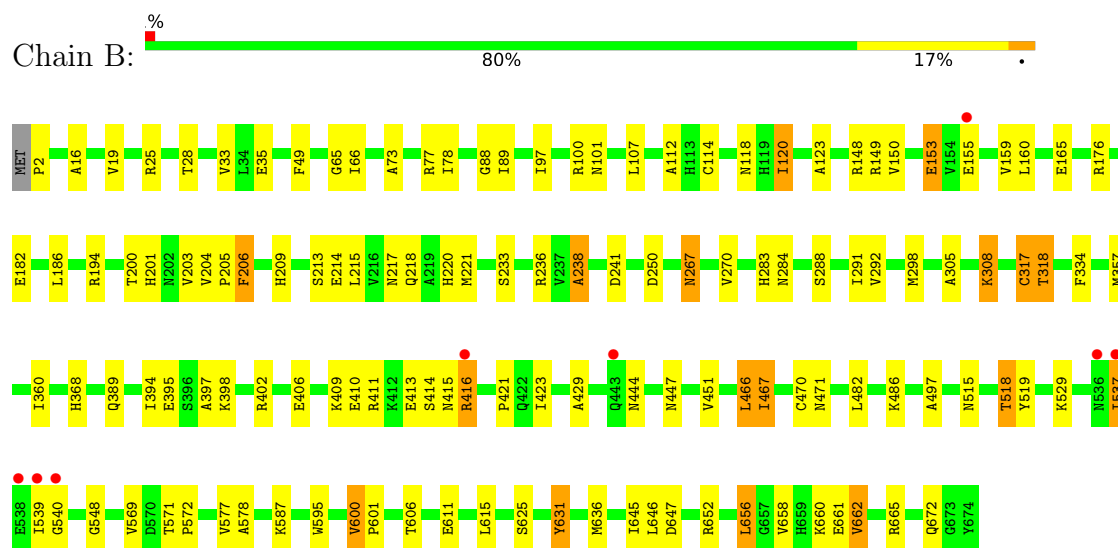
### 3 Residue-property plots

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.

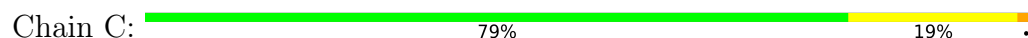
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

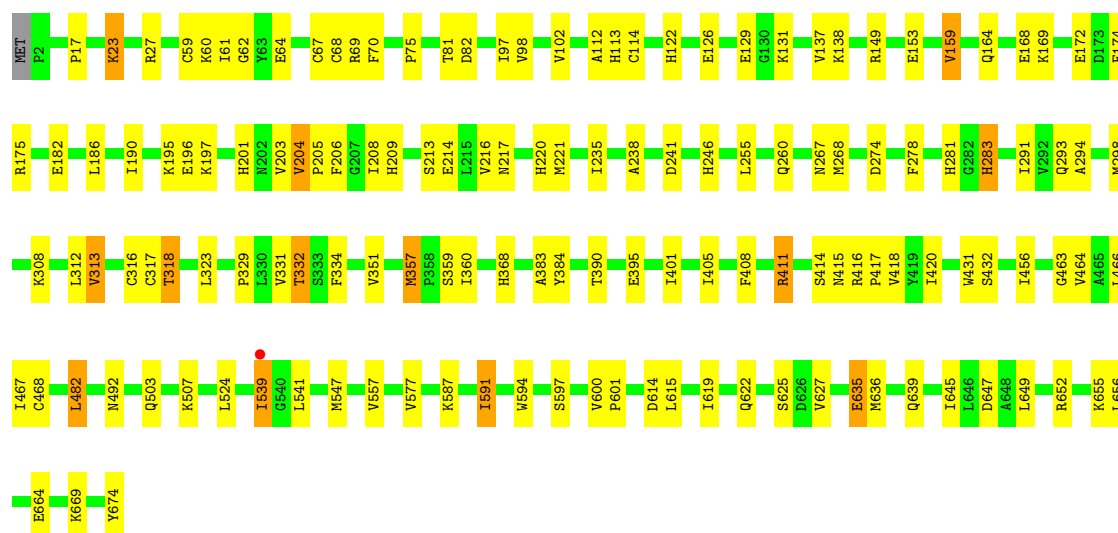


- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta



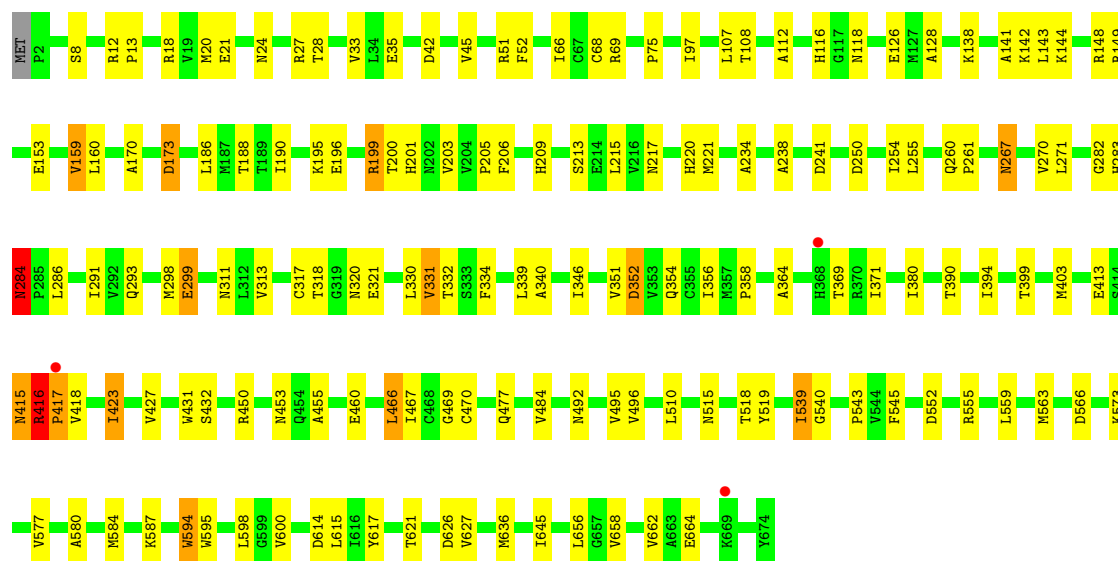
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta





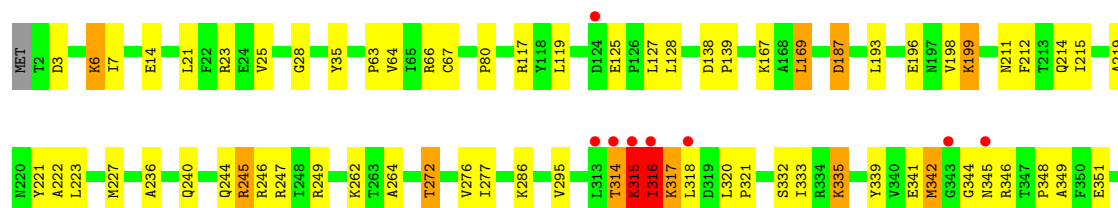
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

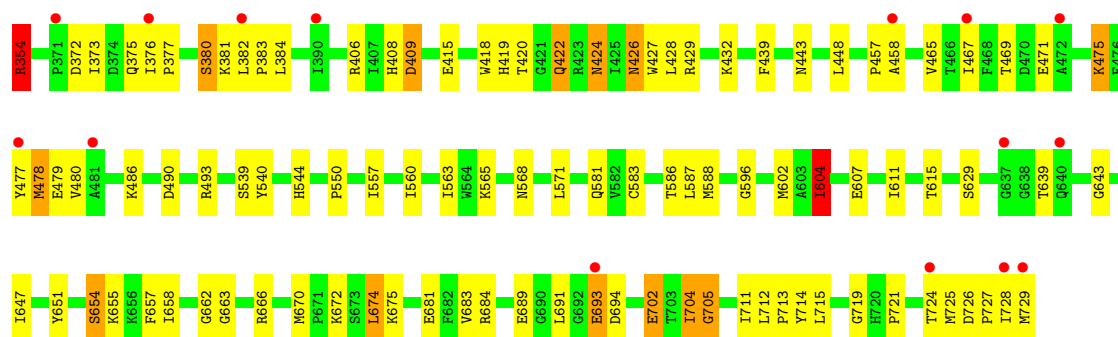
Chain D: 77% 21% .



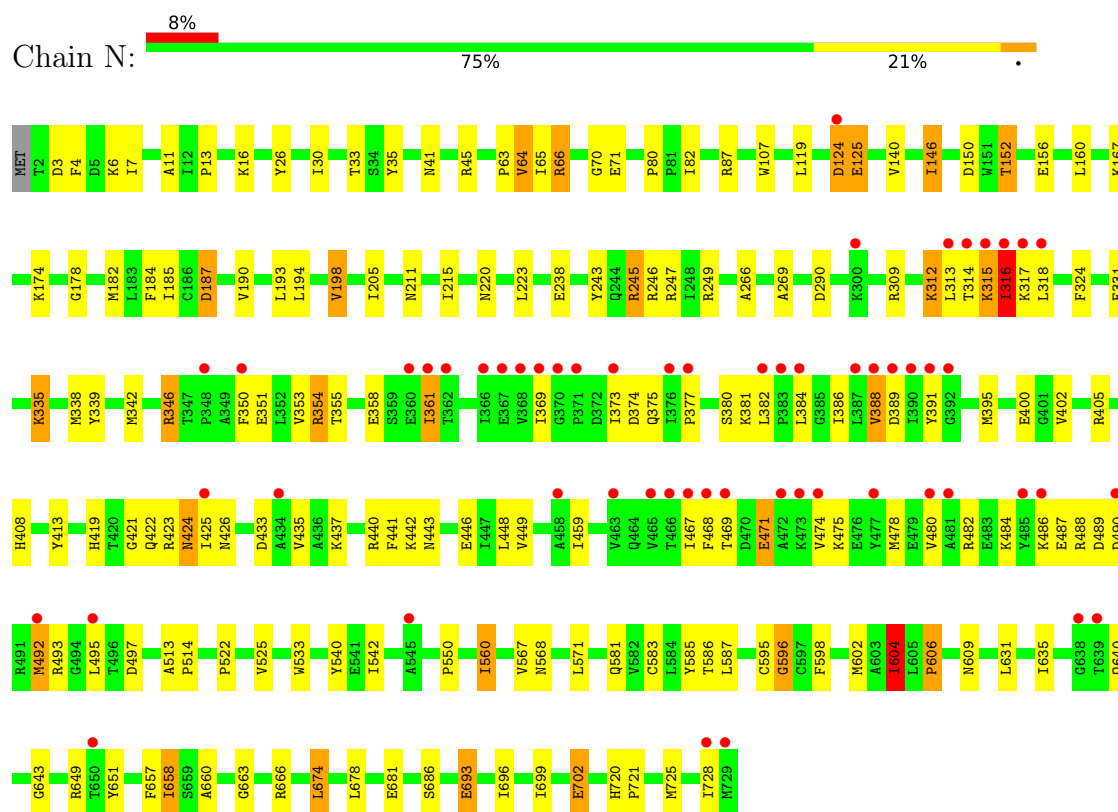
- Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

Chain M: 3% 76% 20% . .

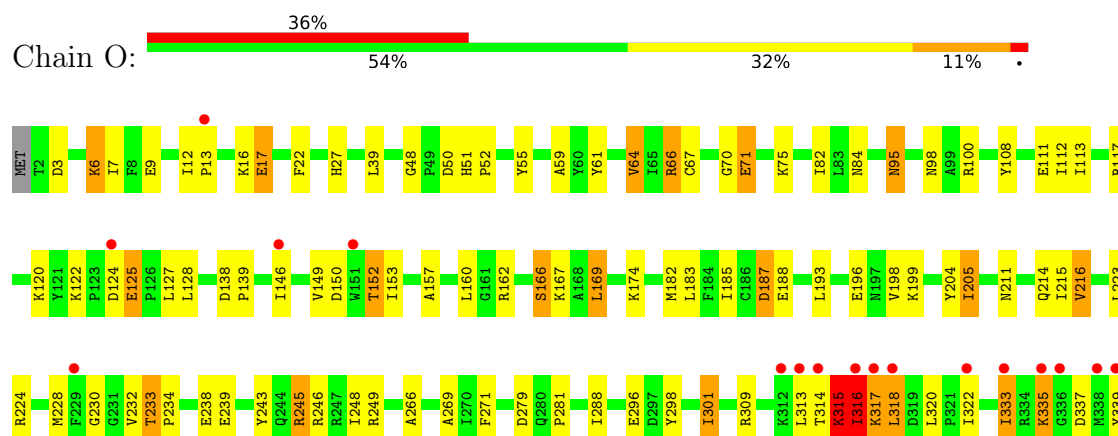


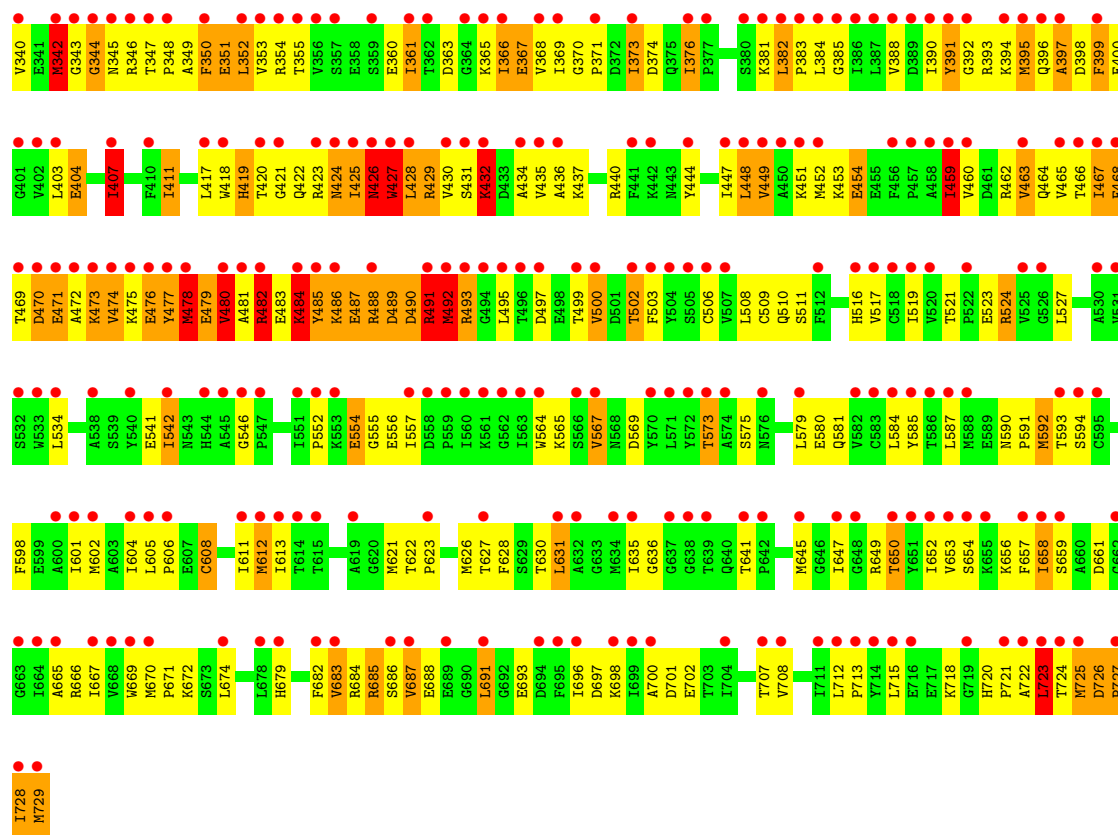


• Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

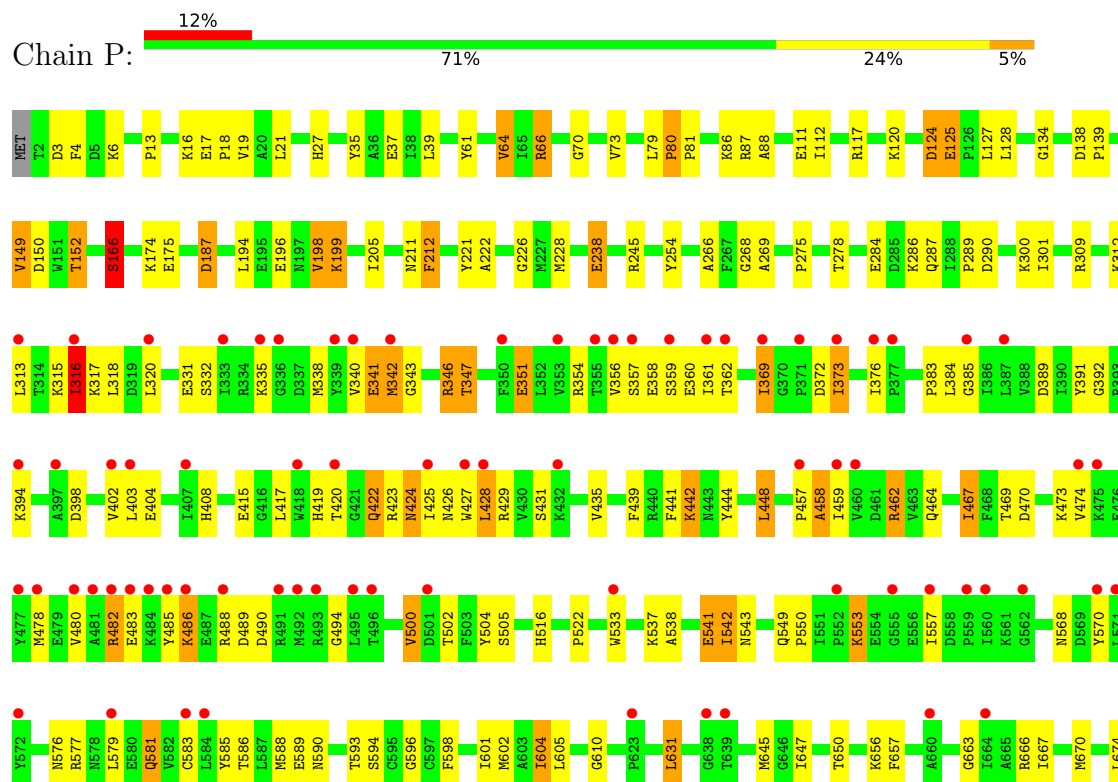


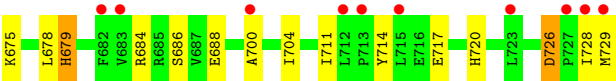
• Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha





- 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, $\alpha$ , $\beta$ , $\gamma$                | 99.65Å 136.87Å 140.86Å<br>101.26° 109.11° 104.08°           | Depositor        |
| Resolution (Å)                                                          | 36.96 – 2.15<br>36.96 – 2.15                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 92.3 (36.96-2.15)<br>92.3 (36.96-2.15)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.07                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.33 (at 2.16Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0019                                             | Depositor        |
| R, $R_{free}$                                                           | 0.186 , 0.242<br>0.187 , 0.240                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 16243 reflections (4.97%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 29.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.301                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 45.5                                                 | 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                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 45096                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 36.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: CU1, XCC, SF4, ACT, NI, GOL, NA

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     | 1.35         | 9/5244 (0.2%)   | 1.24        | 13/7106 (0.2%)   |
| 1   | B     | 1.41         | 18/5231 (0.3%)  | 1.27        | 28/7086 (0.4%)   |
| 1   | C     | 1.35         | 21/5193 (0.4%)  | 1.24        | 16/7038 (0.2%)   |
| 1   | D     | 1.22         | 8/5212 (0.2%)   | 1.22        | 17/7062 (0.2%)   |
| 2   | M     | 1.22         | 10/5921 (0.2%)  | 1.19        | 19/8015 (0.2%)   |
| 2   | N     | 1.24         | 11/5928 (0.2%)  | 1.22        | 23/8023 (0.3%)   |
| 2   | O     | 1.14         | 13/5883 (0.2%)  | 1.29        | 49/7965 (0.6%)   |
| 2   | P     | 1.07         | 6/5885 (0.1%)   | 1.15        | 13/7968 (0.2%)   |
| All | All   | 1.25         | 96/44497 (0.2%) | 1.23        | 178/60263 (0.3%) |

All (96) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | O     | 725 | MET  | C-O    | -9.29 | 1.12        | 1.24     |
| 2   | O     | 478 | MET  | CA-C   | 8.62  | 1.64        | 1.52     |
| 2   | P     | 316 | ILE  | C-N    | -7.73 | 1.23        | 1.33     |
| 1   | C     | 415 | ASN  | C-O    | -7.57 | 1.12        | 1.23     |
| 2   | N     | 107 | TRP  | C-O    | -7.50 | 1.15        | 1.24     |
| 1   | C     | 415 | ASN  | N-CA   | -7.39 | 1.35        | 1.46     |
| 1   | C     | 417 | PRO  | C-O    | -7.19 | 1.14        | 1.23     |
| 1   | C     | 415 | ASN  | CA-C   | -7.02 | 1.43        | 1.53     |
| 1   | D     | 311 | ASN  | CA-C   | 6.96  | 1.61        | 1.53     |
| 1   | B     | 89  | ILE  | CA-CB  | 6.91  | 1.64        | 1.54     |
| 1   | B     | 578 | ALA  | CA-CB  | -6.75 | 1.42        | 1.53     |
| 2   | O     | 419 | HIS  | CG-ND1 | -6.70 | 1.30        | 1.38     |
| 1   | A     | 370 | ARG  | N-CA   | -6.67 | 1.38        | 1.46     |
| 1   | D     | 415 | ASN  | N-CA   | -6.64 | 1.38        | 1.46     |
| 1   | B     | 120 | ILE  | C-O    | -6.63 | 1.16        | 1.24     |
| 2   | N     | 475 | LYS  | N-CA   | -6.63 | 1.37        | 1.46     |
| 1   | C     | 291 | ILE  | CA-CB  | 6.56  | 1.62        | 1.54     |
| 1   | D     | 346 | ILE  | CA-CB  | 6.48  | 1.61        | 1.54     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | O     | 153 | ILE  | CA-CB   | 6.45  | 1.60        | 1.53     |
| 1   | C     | 246 | HIS  | C-O     | -6.39 | 1.16        | 1.24     |
| 1   | C     | 137 | VAL  | CA-CB   | 6.36  | 1.60        | 1.53     |
| 1   | C     | 159 | VAL  | CA-CB   | 6.32  | 1.62        | 1.54     |
| 1   | C     | 332 | THR  | CA-CB   | 6.31  | 1.62        | 1.53     |
| 1   | B     | 236 | ARG  | CA-C    | 6.30  | 1.60        | 1.52     |
| 2   | O     | 419 | HIS  | ND1-CE1 | -6.22 | 1.26        | 1.32     |
| 2   | P     | 212 | PHE  | C-O     | -6.16 | 1.18        | 1.24     |
| 2   | O     | 288 | ILE  | N-CA    | 6.14  | 1.50        | 1.45     |
| 1   | B     | 537 | ILE  | CA-CB   | 6.12  | 1.60        | 1.53     |
| 2   | M     | 264 | ALA  | CA-C    | 6.11  | 1.60        | 1.52     |
| 1   | C     | 464 | VAL  | CA-CB   | 6.09  | 1.62        | 1.54     |
| 1   | A     | 464 | VAL  | CA-CB   | 6.09  | 1.61        | 1.54     |
| 1   | B     | 100 | ARG  | C-O     | -6.09 | 1.17        | 1.24     |
| 1   | C     | 635 | GLU  | N-CA    | 6.08  | 1.53        | 1.46     |
| 2   | N     | 140 | VAL  | CA-CB   | 6.06  | 1.62        | 1.54     |
| 2   | O     | 419 | HIS  | CD2-NE2 | -6.06 | 1.31        | 1.37     |
| 1   | B     | 19  | VAL  | C-O     | -6.04 | 1.17        | 1.24     |
| 2   | O     | 426 | ASN  | CA-C    | -6.01 | 1.44        | 1.53     |
| 1   | D     | 484 | VAL  | CA-CB   | 6.01  | 1.61        | 1.54     |
| 1   | D     | 203 | VAL  | CA-CB   | 5.99  | 1.61        | 1.54     |
| 2   | O     | 427 | TRP  | N-CA    | -5.98 | 1.38        | 1.46     |
| 1   | C     | 318 | THR  | CA-C    | 5.95  | 1.60        | 1.52     |
| 1   | A     | 236 | ARG  | C-O     | -5.93 | 1.17        | 1.24     |
| 1   | B     | 429 | ALA  | CA-CB   | 5.92  | 1.61        | 1.53     |
| 1   | B     | 631 | TYR  | C-O     | -5.89 | 1.16        | 1.23     |
| 1   | C     | 541 | LEU  | C-O     | -5.86 | 1.16        | 1.24     |
| 1   | C     | 203 | VAL  | N-CA    | 5.83  | 1.52        | 1.46     |
| 2   | N     | 525 | VAL  | CA-CB   | 5.79  | 1.62        | 1.54     |
| 1   | A     | 214 | GLU  | C-O     | -5.79 | 1.17        | 1.24     |
| 2   | N     | 65  | ILE  | CA-CB   | -5.74 | 1.47        | 1.54     |
| 1   | D     | 394 | ILE  | CA-CB   | 5.72  | 1.61        | 1.54     |
| 1   | A     | 61  | ILE  | CA-CB   | 5.60  | 1.60        | 1.54     |
| 2   | P     | 80  | PRO  | CA-C    | 5.54  | 1.57        | 1.52     |
| 2   | N     | 87  | ARG  | CA-C    | 5.54  | 1.59        | 1.52     |
| 1   | B     | 194 | ARG  | N-CA    | 5.53  | 1.53        | 1.46     |
| 2   | M     | 467 | ILE  | CA-CB   | 5.48  | 1.60        | 1.53     |
| 1   | D     | 318 | THR  | CA-C    | 5.47  | 1.59        | 1.52     |
| 2   | M     | 639 | THR  | CA-C    | 5.47  | 1.59        | 1.52     |
| 1   | C     | 283 | HIS  | N-CA    | 5.45  | 1.52        | 1.46     |
| 1   | B     | 658 | VAL  | CA-CB   | 5.45  | 1.60        | 1.54     |
| 2   | P     | 198 | VAL  | CA-CB   | 5.43  | 1.60        | 1.54     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 150 | VAL  | C-O   | -5.42 | 1.17        | 1.24     |
| 2   | N     | 190 | VAL  | CA-CB | 5.41  | 1.60        | 1.54     |
| 2   | O     | 683 | VAL  | CA-CB | 5.38  | 1.61        | 1.54     |
| 2   | M     | 221 | TYR  | C-O   | -5.34 | 1.17        | 1.24     |
| 2   | N     | 64  | VAL  | C-O   | -5.34 | 1.18        | 1.24     |
| 2   | N     | 595 | CYS  | CA-C  | 5.32  | 1.57        | 1.53     |
| 1   | B     | 176 | ARG  | C-O   | -5.32 | 1.17        | 1.23     |
| 1   | D     | 352 | ASP  | CA-C  | 5.32  | 1.55        | 1.52     |
| 2   | M     | 28  | GLY  | N-CA  | 5.27  | 1.52        | 1.45     |
| 2   | O     | 687 | VAL  | CA-CB | 5.26  | 1.60        | 1.54     |
| 1   | A     | 89  | ILE  | N-CA  | -5.26 | 1.40        | 1.46     |
| 2   | M     | 465 | VAL  | CA-CB | 5.26  | 1.62        | 1.54     |
| 2   | O     | 685 | ARG  | C-N   | 5.26  | 1.40        | 1.33     |
| 1   | C     | 313 | VAL  | C-O   | -5.25 | 1.18        | 1.23     |
| 1   | A     | 165 | GLU  | CA-C  | 5.21  | 1.59        | 1.52     |
| 1   | C     | 17  | PRO  | C-O   | 5.21  | 1.29        | 1.23     |
| 2   | P     | 73  | VAL  | C-O   | 5.18  | 1.29        | 1.24     |
| 2   | O     | 685 | ARG  | CA-CB | -5.17 | 1.45        | 1.53     |
| 1   | B     | 165 | GLU  | C-O   | -5.16 | 1.18        | 1.24     |
| 1   | C     | 420 | ILE  | CA-CB | 5.16  | 1.59        | 1.53     |
| 1   | A     | 420 | ILE  | CA-C  | 5.15  | 1.57        | 1.53     |
| 1   | B     | 214 | GLU  | CA-C  | 5.11  | 1.59        | 1.52     |
| 1   | A     | 194 | ARG  | N-CA  | 5.08  | 1.52        | 1.46     |
| 1   | B     | 123 | ALA  | N-CA  | -5.08 | 1.39        | 1.46     |
| 2   | M     | 25  | VAL  | CA-CB | 5.07  | 1.60        | 1.54     |
| 1   | C     | 332 | THR  | C-O   | 5.07  | 1.28        | 1.24     |
| 1   | C     | 334 | PHE  | CA-C  | 5.06  | 1.59        | 1.52     |
| 2   | N     | 475 | LYS  | C-O   | -5.05 | 1.17        | 1.24     |
| 1   | C     | 524 | LEU  | CA-C  | 5.04  | 1.59        | 1.52     |
| 2   | N     | 33  | THR  | CA-CB | 5.03  | 1.61        | 1.53     |
| 2   | M     | 629 | SER  | N-CA  | 5.02  | 1.52        | 1.46     |
| 2   | P     | 650 | THR  | CA-CB | 5.02  | 1.61        | 1.53     |
| 2   | M     | 639 | THR  | CA-CB | 5.02  | 1.61        | 1.53     |
| 1   | B     | 238 | ALA  | CA-CB | 5.01  | 1.61        | 1.53     |
| 2   | M     | 604 | ILE  | CA-CB | 5.01  | 1.59        | 1.54     |
| 1   | B     | 203 | VAL  | CA-CB | 5.00  | 1.61        | 1.54     |

All (178) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | O     | 480 | VAL  | N-CA-C | -12.86 | 99.04       | 110.74   |
| 2   | O     | 476 | GLU  | N-CA-C | -11.60 | 98.64       | 111.28   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2   | O     | 479 | GLU  | N-CA-C      | -10.78 | 99.23       | 112.38   |
| 2   | O     | 473 | LYS  | N-CA-C      | 10.26  | 122.54      | 111.36   |
| 2   | O     | 723 | LEU  | N-CA-C      | 9.77   | 121.53      | 111.07   |
| 2   | O     | 474 | VAL  | N-CA-C      | -9.57  | 99.09       | 111.05   |
| 1   | A     | 344 | GLY  | N-CA-C      | -9.21  | 103.24      | 115.21   |
| 2   | O     | 471 | GLU  | N-CA-C      | 8.80   | 120.96      | 111.36   |
| 2   | O     | 554 | GLU  | N-CA-C      | 8.55   | 122.84      | 109.07   |
| 1   | A     | 574 | VAL  | N-CA-C      | 8.14   | 115.63      | 108.63   |
| 2   | O     | 419 | HIS  | ND1-CE1-NE2 | 7.96   | 116.36      | 108.40   |
| 2   | O     | 726 | ASP  | N-CA-C      | 7.88   | 122.21      | 110.39   |
| 2   | N     | 728 | ILE  | N-CA-C      | -7.79  | 103.32      | 111.58   |
| 2   | O     | 344 | GLY  | N-CA-C      | 7.63   | 127.50      | 113.76   |
| 2   | P     | 86  | LYS  | N-CA-C      | 7.55   | 119.59      | 111.36   |
| 2   | O     | 477 | TYR  | N-CA-C      | 7.54   | 119.57      | 111.36   |
| 1   | B     | 548 | GLY  | N-CA-C      | 7.46   | 119.09      | 111.56   |
| 1   | B     | 317 | CYS  | N-CA-C      | 7.45   | 119.48      | 111.36   |
| 2   | M     | 128 | LEU  | CA-C-N      | -7.42  | 112.74      | 120.38   |
| 2   | M     | 128 | LEU  | C-N-CA      | -7.42  | 112.74      | 120.38   |
| 2   | N     | 720 | HIS  | CA-C-N      | 7.39   | 127.10      | 119.56   |
| 2   | N     | 720 | HIS  | C-N-CA      | 7.39   | 127.10      | 119.56   |
| 2   | O     | 419 | HIS  | ND1-CG-CD2  | 7.25   | 113.35      | 106.10   |
| 2   | O     | 478 | MET  | CA-C-N      | 7.18   | 132.10      | 120.60   |
| 2   | O     | 478 | MET  | C-N-CA      | 7.18   | 132.10      | 120.60   |
| 2   | N     | 513 | ALA  | CA-C-N      | 7.12   | 127.44      | 119.32   |
| 2   | N     | 513 | ALA  | C-N-CA      | 7.12   | 127.44      | 119.32   |
| 1   | B     | 120 | ILE  | N-CA-C      | 7.08   | 117.22      | 110.42   |
| 1   | B     | 101 | ASN  | N-CA-C      | 7.08   | 118.78      | 111.14   |
| 2   | P     | 316 | ILE  | N-CA-C      | 7.07   | 124.05      | 109.34   |
| 1   | D     | 416 | ARG  | N-CA-C      | 7.02   | 125.33      | 109.81   |
| 2   | O     | 685 | ARG  | N-CA-CB     | -7.00  | 99.83       | 110.12   |
| 2   | N     | 382 | LEU  | CA-C-N      | -6.99  | 113.46      | 120.31   |
| 2   | N     | 382 | LEU  | C-N-CA      | -6.99  | 113.46      | 120.31   |
| 1   | C     | 334 | PHE  | N-CA-C      | 6.87   | 119.40      | 111.02   |
| 1   | B     | 318 | THR  | N-CA-C      | -6.83  | 103.91      | 111.36   |
| 2   | N     | 567 | VAL  | N-CA-C      | -6.80  | 103.58      | 111.00   |
| 2   | O     | 491 | ARG  | N-CA-C      | -6.78  | 95.62       | 108.17   |
| 1   | C     | 357 | MET  | CA-C-N      | -6.69  | 112.70      | 120.12   |
| 1   | C     | 357 | MET  | C-N-CA      | -6.69  | 112.70      | 120.12   |
| 2   | O     | 407 | ILE  | N-CA-C      | -6.68  | 106.49      | 111.90   |
| 2   | M     | 80  | PRO  | N-CA-C      | 6.67   | 118.84      | 110.70   |
| 2   | O     | 490 | ASP  | N-CA-C      | 6.64   | 124.95      | 110.80   |
| 2   | O     | 301 | ILE  | N-CA-C      | 6.64   | 116.79      | 110.42   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | N     | 361 | ILE  | N-CA-C  | 6.63  | 117.85      | 108.17   |
| 2   | O     | 478 | MET  | N-CA-C  | 6.61  | 124.89      | 110.80   |
| 2   | M     | 705 | GLY  | N-CA-C  | 6.60  | 120.25      | 110.42   |
| 2   | O     | 427 | TRP  | N-CA-CB | -6.54 | 100.83      | 111.24   |
| 1   | A     | 470 | CYS  | N-CA-C  | 6.52  | 119.34      | 109.63   |
| 1   | D     | 580 | ALA  | CA-C-N  | 6.50  | 126.19      | 119.56   |
| 1   | D     | 580 | ALA  | C-N-CA  | 6.50  | 126.19      | 119.56   |
| 1   | C     | 411 | ARG  | N-CA-C  | -6.48 | 104.14      | 111.14   |
| 2   | N     | 604 | ILE  | CB-CA-C | -6.47 | 101.57      | 111.08   |
| 1   | B     | 284 | ASN  | N-CA-C  | 6.46  | 118.22      | 109.24   |
| 2   | O     | 342 | MET  | N-CA-C  | 6.42  | 118.82      | 109.07   |
| 2   | P     | 268 | GLY  | N-CA-C  | -6.37 | 104.31      | 113.86   |
| 2   | O     | 546 | GLY  | CA-C-N  | 6.36  | 125.93      | 119.19   |
| 2   | O     | 546 | GLY  | C-N-CA  | 6.36  | 125.93      | 119.19   |
| 2   | O     | 233 | THR  | CB-CA-C | -6.31 | 99.26       | 109.67   |
| 2   | M     | 384 | LEU  | N-CA-C  | 6.22  | 119.39      | 108.75   |
| 1   | B     | 611 | GLU  | N-CA-C  | 6.17  | 118.80      | 111.71   |
| 2   | O     | 573 | THR  | N-CA-C  | 6.16  | 119.26      | 111.69   |
| 2   | M     | 316 | ILE  | N-CA-C  | 6.10  | 122.03      | 109.34   |
| 2   | O     | 682 | PHE  | N-CA-C  | 6.08  | 117.99      | 111.36   |
| 1   | A     | 283 | HIS  | N-CA-C  | 6.08  | 121.55      | 114.62   |
| 1   | A     | 150 | VAL  | N-CA-C  | 6.08  | 117.32      | 111.91   |
| 1   | D     | 495 | VAL  | N-CA-C  | 6.02  | 116.97      | 108.36   |
| 2   | N     | 346 | ARG  | N-CA-C  | -6.02 | 104.68      | 112.68   |
| 1   | D     | 141 | ALA  | N-CA-C  | -5.89 | 104.77      | 111.07   |
| 2   | O     | 48  | GLY  | CA-C-N  | 5.89  | 125.57      | 119.56   |
| 2   | O     | 48  | GLY  | C-N-CA  | 5.89  | 125.57      | 119.56   |
| 1   | D     | 539 | ILE  | N-CA-C  | 5.88  | 121.56      | 109.34   |
| 2   | M     | 689 | GLU  | N-CA-C  | -5.87 | 106.16      | 113.38   |
| 1   | B     | 357 | MET  | CA-C-N  | -5.87 | 113.94      | 120.45   |
| 1   | B     | 357 | MET  | C-N-CA  | -5.87 | 113.94      | 120.45   |
| 1   | C     | 283 | HIS  | N-CA-C  | 5.86  | 121.30      | 114.62   |
| 1   | D     | 42  | ASP  | N-CA-C  | 5.82  | 117.30      | 111.07   |
| 2   | P     | 128 | LEU  | CA-C-N  | 5.82  | 126.37      | 120.38   |
| 2   | P     | 128 | LEU  | C-N-CA  | 5.82  | 126.37      | 120.38   |
| 2   | N     | 314 | THR  | CB-CA-C | -5.80 | 98.87       | 110.42   |
| 2   | O     | 128 | LEU  | CA-C-N  | -5.79 | 114.42      | 120.38   |
| 2   | O     | 128 | LEU  | C-N-CA  | -5.79 | 114.42      | 120.38   |
| 2   | O     | 725 | MET  | N-CA-C  | -5.79 | 98.48       | 110.80   |
| 2   | O     | 426 | ASN  | CB-CA-C | -5.77 | 99.51       | 113.19   |
| 1   | D     | 519 | TYR  | N-CA-C  | 5.76  | 120.96      | 113.88   |
| 2   | P     | 134 | GLY  | N-CA-C  | -5.73 | 101.81      | 111.73   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | M     | 276 | VAL  | CA-C-N   | -5.72 | 115.65      | 123.14   |
| 2   | M     | 276 | VAL  | C-N-CA   | -5.72 | 115.65      | 123.14   |
| 1   | B     | 416 | ARG  | CA-C-N   | -5.71 | 114.38      | 120.03   |
| 1   | B     | 416 | ARG  | C-N-CA   | -5.71 | 114.38      | 120.03   |
| 2   | M     | 557 | ILE  | N-CA-C   | -5.66 | 107.32      | 111.90   |
| 1   | B     | 600 | VAL  | N-CA-CB  | -5.65 | 103.30      | 111.21   |
| 1   | A     | 81  | THR  | N-CA-C   | -5.59 | 106.45      | 113.28   |
| 1   | B     | 334 | PHE  | N-CA-C   | 5.58  | 117.83      | 111.02   |
| 2   | M     | 691 | LEU  | N-CA-C   | -5.57 | 106.84      | 113.97   |
| 1   | B     | 470 | CYS  | N-CA-C   | 5.56  | 118.46      | 109.79   |
| 1   | A     | 191 | ASN  | N-CA-C   | 5.55  | 117.23      | 110.41   |
| 2   | O     | 84  | ASN  | N-CA-C   | 5.55  | 117.33      | 111.28   |
| 1   | B     | 16  | ALA  | CA-C-N   | -5.54 | 114.25      | 119.85   |
| 1   | B     | 16  | ALA  | C-N-CA   | -5.54 | 114.25      | 119.85   |
| 1   | D     | 334 | PHE  | N-CA-C   | 5.50  | 117.73      | 111.02   |
| 2   | O     | 468 | PHE  | N-CA-C   | 5.50  | 117.75      | 109.23   |
| 1   | B     | 206 | PHE  | CA-C-N   | 5.46  | 125.82      | 121.61   |
| 1   | B     | 206 | PHE  | C-N-CA   | 5.46  | 125.82      | 121.61   |
| 1   | A     | 269 | GLY  | N-CA-C   | -5.46 | 108.17      | 115.32   |
| 1   | B     | 662 | VAL  | N-CA-C   | 5.46  | 115.66      | 110.42   |
| 1   | D     | 159 | VAL  | N-CA-CB  | 5.45  | 118.75      | 110.58   |
| 2   | N     | 318 | LEU  | CA-C-N   | -5.43 | 115.11      | 122.77   |
| 2   | N     | 318 | LEU  | C-N-CA   | -5.43 | 115.11      | 122.77   |
| 1   | B     | 471 | ASN  | N-CA-C   | -5.42 | 101.74      | 110.14   |
| 2   | M     | 354 | ARG  | N-CA-C   | 5.41  | 117.49      | 108.99   |
| 2   | O     | 517 | VAL  | N-CA-C   | 5.41  | 115.84      | 107.78   |
| 1   | B     | 600 | VAL  | CA-C-N   | -5.39 | 114.37      | 119.76   |
| 1   | B     | 600 | VAL  | C-N-CA   | -5.39 | 114.37      | 119.76   |
| 1   | C     | 539 | ILE  | N-CA-C   | 5.37  | 117.80      | 111.09   |
| 2   | M     | 666 | ARG  | N-CA-C   | 5.35  | 119.06      | 112.54   |
| 2   | O     | 301 | ILE  | CB-CA-C  | -5.33 | 105.14      | 111.97   |
| 1   | A     | 594 | TRP  | CA-CB-CG | 5.33  | 123.73      | 113.60   |
| 2   | O     | 12  | ILE  | CA-C-N   | 5.33  | 126.50      | 119.84   |
| 2   | O     | 12  | ILE  | C-N-CA   | 5.33  | 126.50      | 119.84   |
| 1   | C     | 492 | ASN  | N-CA-C   | 5.29  | 119.02      | 112.24   |
| 2   | N     | 702 | GLU  | CB-CA-C  | -5.29 | 99.16       | 110.32   |
| 1   | D     | 173 | ASP  | N-CA-C   | -5.26 | 106.37      | 112.89   |
| 1   | C     | 432 | SER  | N-CA-C   | -5.25 | 103.95      | 110.41   |
| 2   | N     | 119 | LEU  | N-CA-C   | -5.24 | 105.99      | 112.38   |
| 2   | P     | 604 | ILE  | N-CA-C   | 5.23  | 116.33      | 109.58   |
| 1   | A     | 120 | ILE  | N-CA-C   | 5.22  | 115.94      | 110.62   |
| 1   | A     | 186 | LEU  | N-CA-C   | -5.21 | 104.53      | 112.04   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | M     | 222 | ALA  | N-CA-C  | 5.21  | 119.97      | 111.37   |
| 2   | P     | 19  | VAL  | N-CA-C  | 5.19  | 115.96      | 110.72   |
| 2   | M     | 119 | LEU  | N-CA-C  | -5.18 | 105.75      | 111.71   |
| 2   | O     | 424 | ASN  | N-CA-C  | 5.18  | 116.93      | 111.28   |
| 2   | N     | 41  | ASN  | N-CA-C  | 5.18  | 117.01      | 111.36   |
| 2   | P     | 37  | GLU  | N-CA-C  | 5.17  | 116.60      | 111.07   |
| 2   | P     | 720 | HIS  | CA-C-N  | 5.17  | 126.30      | 119.84   |
| 2   | P     | 720 | HIS  | C-N-CA  | 5.17  | 126.30      | 119.84   |
| 2   | O     | 449 | VAL  | N-CA-C  | 5.16  | 115.82      | 110.82   |
| 1   | A     | 111 | ALA  | N-CA-C  | 5.15  | 116.90      | 111.28   |
| 1   | C     | 175 | ARG  | N-CA-C  | 5.15  | 118.72      | 112.23   |
| 2   | N     | 80  | PRO  | CA-C-N  | -5.15 | 113.73      | 119.19   |
| 2   | N     | 80  | PRO  | C-N-CA  | -5.15 | 113.73      | 119.19   |
| 2   | O     | 432 | LYS  | N-CA-C  | -5.15 | 105.67      | 111.28   |
| 1   | D     | 417 | PRO  | N-CA-C  | -5.14 | 102.88      | 111.26   |
| 2   | O     | 67  | CYS  | N-CA-C  | 5.13  | 116.56      | 110.97   |
| 1   | A     | 321 | GLU  | N-CA-C  | 5.12  | 117.26      | 111.11   |
| 1   | B     | 120 | ILE  | CA-C-O  | -5.12 | 115.74      | 121.17   |
| 1   | D     | 371 | ILE  | N-CA-C  | -5.12 | 101.04      | 108.36   |
| 1   | C     | 159 | VAL  | N-CA-CB | 5.11  | 117.49      | 110.54   |
| 1   | D     | 8   | SER  | CA-C-N  | -5.11 | 116.19      | 122.84   |
| 1   | D     | 8   | SER  | C-N-CA  | -5.11 | 116.19      | 122.84   |
| 2   | O     | 55  | TYR  | CA-C-N  | -5.11 | 115.46      | 120.52   |
| 2   | O     | 55  | TYR  | C-N-CA  | -5.11 | 115.46      | 120.52   |
| 2   | N     | 3   | ASP  | N-CA-C  | 5.10  | 119.79      | 111.37   |
| 2   | N     | 80  | PRO  | N-CA-C  | 5.09  | 116.91      | 110.70   |
| 2   | M     | 604 | ILE  | CB-CA-C | -5.09 | 103.60      | 111.08   |
| 1   | D     | 284 | ASN  | N-CA-C  | 5.08  | 116.31      | 109.24   |
| 1   | B     | 394 | ILE  | N-CA-C  | 5.08  | 115.70      | 110.36   |
| 1   | B     | 646 | LEU  | CA-C-N  | 5.08  | 127.05      | 120.44   |
| 1   | B     | 646 | LEU  | C-N-CA  | 5.08  | 127.05      | 120.44   |
| 1   | C     | 591 | ILE  | N-CA-C  | 5.08  | 115.30      | 110.42   |
| 2   | M     | 63  | PRO  | N-CA-C  | 5.08  | 120.22      | 113.57   |
| 2   | N     | 649 | ARG  | N-CA-C  | 5.08  | 116.81      | 111.28   |
| 2   | M     | 272 | THR  | CB-CA-C | -5.06 | 100.90      | 110.01   |
| 2   | O     | 373 | ILE  | CB-CA-C | 5.06  | 115.51      | 111.06   |
| 1   | B     | 176 | ARG  | N-CA-C  | 5.05  | 117.55      | 110.23   |
| 2   | P     | 166 | SER  | N-CA-C  | 5.05  | 116.79      | 111.28   |
| 1   | C     | 204 | VAL  | CA-C-N  | -5.05 | 114.75      | 119.85   |
| 1   | C     | 204 | VAL  | C-N-CA  | -5.05 | 114.75      | 119.85   |
| 1   | C     | 268 | MET  | N-CA-C  | 5.04  | 118.53      | 112.38   |
| 2   | N     | 316 | ILE  | N-CA-C  | -5.04 | 98.85       | 109.34   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | M     | 662 | GLY  | N-CA-C  | 5.04 | 121.70      | 114.64   |
| 1   | C     | 70  | PHE  | N-CA-C  | 5.04 | 119.06      | 113.01   |
| 2   | O     | 425 | ILE  | N-CA-C  | 5.03 | 114.42      | 106.32   |
| 2   | O     | 472 | ALA  | N-CA-C  | 5.03 | 117.72      | 111.24   |
| 1   | C     | 113 | HIS  | N-CA-C  | 5.03 | 116.76      | 111.28   |
| 1   | D     | 254 | ILE  | N-CA-C  | 5.02 | 115.24      | 110.42   |
| 2   | P     | 149 | VAL  | N-CA-C  | 5.02 | 117.36      | 111.09   |
| 1   | B     | 360 | ILE  | N-CA-CB | 5.01 | 117.36      | 110.54   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5128  | 0        | 5128     | 68      | 0            |
| 1   | B     | 5121  | 0        | 5134     | 75      | 0            |
| 1   | C     | 5094  | 0        | 5097     | 93      | 0            |
| 1   | D     | 5119  | 0        | 5115     | 112     | 0            |
| 2   | M     | 5778  | 0        | 5736     | 104     | 0            |
| 2   | N     | 5784  | 0        | 5749     | 108     | 0            |
| 2   | O     | 5749  | 0        | 5716     | 394     | 0            |
| 2   | P     | 5746  | 0        | 5710     | 151     | 0            |
| 3   | A     | 16    | 0        | 0        | 0       | 0            |
| 3   | B     | 8     | 0        | 0        | 1       | 0            |
| 3   | C     | 16    | 0        | 0        | 1       | 0            |
| 3   | D     | 8     | 0        | 0        | 0       | 0            |
| 3   | M     | 8     | 0        | 0        | 0       | 0            |
| 3   | N     | 8     | 0        | 0        | 1       | 0            |
| 3   | O     | 8     | 0        | 0        | 2       | 0            |
| 3   | P     | 8     | 0        | 0        | 0       | 0            |
| 4   | A     | 9     | 0        | 0        | 1       | 0            |
| 4   | B     | 9     | 0        | 0        | 0       | 0            |
| 4   | C     | 9     | 0        | 0        | 0       | 0            |
| 4   | D     | 9     | 0        | 0        | 2       | 0            |
| 5   | A     | 6     | 0        | 8        | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | B     | 6     | 0        | 7        | 0       | 0            |
| 5   | C     | 6     | 0        | 8        | 5       | 0            |
| 5   | D     | 6     | 0        | 8        | 6       | 0            |
| 6   | M     | 1     | 0        | 0        | 0       | 0            |
| 6   | N     | 1     | 0        | 0        | 0       | 0            |
| 6   | O     | 1     | 0        | 0        | 0       | 0            |
| 6   | P     | 1     | 0        | 0        | 0       | 0            |
| 7   | M     | 1     | 0        | 0        | 0       | 0            |
| 7   | N     | 1     | 0        | 0        | 0       | 0            |
| 7   | O     | 1     | 0        | 0        | 0       | 0            |
| 7   | P     | 1     | 0        | 0        | 0       | 0            |
| 8   | M     | 3     | 0        | 3        | 0       | 0            |
| 8   | N     | 3     | 0        | 3        | 0       | 0            |
| 8   | O     | 3     | 0        | 3        | 1       | 0            |
| 8   | P     | 3     | 0        | 3        | 1       | 0            |
| 9   | M     | 1     | 0        | 0        | 0       | 0            |
| 9   | N     | 1     | 0        | 0        | 0       | 0            |
| 9   | O     | 1     | 0        | 0        | 0       | 0            |
| 9   | P     | 1     | 0        | 0        | 0       | 0            |
| 10  | A     | 215   | 0        | 0        | 5       | 0            |
| 10  | B     | 288   | 0        | 0        | 4       | 0            |
| 10  | C     | 169   | 0        | 0        | 6       | 0            |
| 10  | D     | 151   | 0        | 0        | 4       | 0            |
| 10  | M     | 218   | 0        | 0        | 5       | 0            |
| 10  | N     | 227   | 0        | 0        | 6       | 0            |
| 10  | O     | 27    | 0        | 0        | 2       | 0            |
| 10  | P     | 118   | 0        | 0        | 6       | 0            |
| All | All   | 45096 | 0        | 43428    | 1063    | 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 12.

All (1063) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 2:O:482:ARG:HA  | 2:O:482:ARG:CZ   | 1.72                     | 1.19              |
| 2:P:588:MET:HE1 | 2:P:604:ILE:HD13 | 1.17                     | 1.17              |
| 2:O:490:ASP:HB2 | 2:O:491:ARG:NH1  | 1.61                     | 1.16              |
| 2:O:685:ARG:O   | 2:O:688:GLU:HB3  | 1.44                     | 1.15              |
| 2:O:482:ARG:HA  | 2:O:482:ARG:NH1  | 1.62                     | 1.13              |
| 2:M:602:MET:HE3 | 2:M:647:ILE:HD13 | 1.31                     | 1.13              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 2:M:335:LYS:HD2     | 2:M:335:LYS:H    | 1.07                     | 1.12              |
| 2:O:477:TYR:O       | 2:O:480:VAL:HB   | 1.51                     | 1.10              |
| 2:N:335:LYS:H       | 2:N:335:LYS:CD   | 1.66                     | 1.09              |
| 2:N:335:LYS:HD3     | 2:N:335:LYS:N    | 1.65                     | 1.08              |
| 2:O:490:ASP:HB2     | 2:O:491:ARG:HH12 | 1.09                     | 1.08              |
| 2:M:602:MET:CE      | 2:M:647:ILE:HD13 | 1.84                     | 1.08              |
| 2:O:391:TYR:HD2     | 2:O:462:ARG:HB2  | 1.19                     | 1.07              |
| 2:P:588:MET:CE      | 2:P:604:ILE:HD13 | 1.88                     | 1.04              |
| 2:O:420:THR:OG1     | 2:O:427:TRP:HE3  | 1.38                     | 1.04              |
| 2:O:487:GLU:HG2     | 2:O:488:ARG:N    | 1.67                     | 1.04              |
| 2:O:557:ILE:HD11    | 2:O:565:LYS:HG3  | 1.35                     | 1.03              |
| 2:N:246[B]:ARG:HH12 | 2:N:247:ARG:NH1  | 1.56                     | 1.02              |
| 2:O:427:TRP:C       | 2:O:428:LEU:HD22 | 1.85                     | 1.02              |
| 2:P:444:TYR:O       | 2:P:448:LEU:HD22 | 1.60                     | 1.02              |
| 2:O:371:PRO:HD2     | 2:O:469:THR:OG1  | 1.56                     | 1.01              |
| 2:N:315:LYS:HE2     | 2:N:315:LYS:H    | 1.22                     | 1.01              |
| 2:O:604:ILE:HD12    | 2:O:606:PRO:HD3  | 1.41                     | 1.00              |
| 2:O:483:GLU:O       | 2:O:486:LYS:HB3  | 1.59                     | 1.00              |
| 2:N:335:LYS:H       | 2:N:335:LYS:HD3  | 0.83                     | 1.00              |
| 2:O:466:THR:C       | 2:O:467:ILE:HD12 | 1.86                     | 0.99              |
| 2:O:351:GLU:HG2     | 2:O:423:ARG:H    | 1.27                     | 0.99              |
| 2:O:723:LEU:HD23    | 2:O:723:LEU:C    | 1.86                     | 0.99              |
| 2:O:483:GLU:CG      | 2:O:484:LYS:H    | 1.77                     | 0.97              |
| 2:O:483:GLU:HG3     | 2:O:484:LYS:N    | 1.77                     | 0.96              |
| 2:O:487:GLU:HG2     | 2:O:488:ARG:H    | 1.26                     | 0.96              |
| 2:O:343:GLY:CA      | 2:O:349:ALA:HB2  | 1.95                     | 0.96              |
| 2:O:348:PRO:CB      | 2:O:475:LYS:HE2  | 1.94                     | 0.95              |
| 2:O:487:GLU:CG      | 2:O:488:ARG:N    | 2.30                     | 0.95              |
| 2:O:348:PRO:HB3     | 2:O:475:LYS:HE2  | 1.48                     | 0.95              |
| 2:O:482:ARG:CZ      | 2:O:482:ARG:CA   | 2.44                     | 0.95              |
| 2:O:391:TYR:CD2     | 2:O:462:ARG:HB2  | 2.00                     | 0.95              |
| 2:O:418:TRP:CH2     | 2:O:420:THR:HG21 | 2.02                     | 0.94              |
| 2:O:348:PRO:CG      | 2:O:475:LYS:HE2  | 1.97                     | 0.94              |
| 2:O:418:TRP:CH2     | 2:O:420:THR:CG2  | 2.51                     | 0.93              |
| 1:D:539:ILE:HG23    | 1:D:540:GLY:N    | 1.84                     | 0.92              |
| 2:N:484:LYS:HG2     | 10:N:1375:HOH:O  | 1.68                     | 0.92              |
| 2:O:418:TRP:CZ3     | 2:O:420:THR:HG23 | 2.05                     | 0.92              |
| 2:O:351:GLU:HB2     | 2:O:426:ASN:ND2  | 1.85                     | 0.92              |
| 2:M:335:LYS:HD2     | 2:M:335:LYS:N    | 1.86                     | 0.91              |
| 2:P:13:PRO:HB2      | 2:P:16:LYS:HG3   | 1.53                     | 0.91              |
| 2:O:367:GLU:OE2     | 2:O:369:ILE:HD11 | 1.69                     | 0.90              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 2:O:483:GLU:CG      | 2:O:484:LYS:N    | 2.30                     | 0.90              |
| 2:P:602:MET:CE      | 2:P:647:ILE:HG21 | 2.02                     | 0.90              |
| 2:O:370:GLY:HA3     | 2:O:469:THR:HG1  | 1.38                     | 0.88              |
| 2:M:341:GLU:OE1     | 2:M:381:LYS:HE3  | 1.73                     | 0.87              |
| 2:O:480:VAL:O       | 2:O:483:GLU:HG2  | 1.74                     | 0.87              |
| 2:N:315:LYS:HE2     | 2:N:315:LYS:N    | 1.90                     | 0.87              |
| 2:O:376:ILE:HG21    | 2:O:382:LEU:HD21 | 1.56                     | 0.86              |
| 2:O:351:GLU:HB3     | 2:O:423:ARG:N    | 1.89                     | 0.86              |
| 2:O:351:GLU:CG      | 2:O:423:ARG:H    | 1.88                     | 0.86              |
| 1:D:416:ARG:O       | 1:D:418:VAL:HG23 | 1.76                     | 0.86              |
| 2:M:335:LYS:H       | 2:M:335:LYS:CD   | 1.88                     | 0.86              |
| 2:O:666:ARG:NH2     | 2:O:725:MET:HE2  | 1.90                     | 0.85              |
| 2:O:157:ALA:HB3     | 2:O:183:LEU:CD2  | 2.05                     | 0.85              |
| 2:O:715:LEU:HD22    | 2:O:720:HIS:HD2  | 1.40                     | 0.85              |
| 2:P:470:ASP:HA      | 10:P:1362:HOH:O  | 1.75                     | 0.85              |
| 2:P:342:MET:HG3     | 2:P:384:LEU:HD22 | 1.56                     | 0.85              |
| 2:O:653:VAL:O       | 2:O:685:ARG:HD2  | 1.77                     | 0.84              |
| 2:O:370:GLY:HA3     | 2:O:469:THR:OG1  | 1.79                     | 0.83              |
| 2:O:685:ARG:NH1     | 2:O:685:ARG:HB3  | 1.93                     | 0.83              |
| 2:O:350:PHE:CD2     | 2:O:385:GLY:HA3  | 2.14                     | 0.82              |
| 2:O:365:LYS:HG2     | 2:O:464:GLN:HG3  | 1.60                     | 0.82              |
| 2:O:418:TRP:CZ3     | 2:O:420:THR:CG2  | 2.62                     | 0.82              |
| 2:P:4:PHE:HB2       | 2:P:238:GLU:OE2  | 1.79                     | 0.82              |
| 5:D:863:GOL:H2      | 2:P:27:HIS:HE1   | 1.43                     | 0.82              |
| 2:O:723:LEU:HD23    | 2:O:723:LEU:O    | 1.79                     | 0.82              |
| 2:O:396:GLN:HG3     | 2:O:399:PHE:CD1  | 2.15                     | 0.81              |
| 2:P:150:ASP:OD2     | 2:P:152:THR:HG22 | 1.79                     | 0.81              |
| 5:C:863:GOL:H31     | 2:O:27:HIS:CE1   | 2.15                     | 0.81              |
| 2:O:419:HIS:HE1     | 2:O:421:GLY:O    | 1.64                     | 0.80              |
| 1:D:68:CYS:HB2      | 1:D:97:ILE:HG23  | 1.61                     | 0.80              |
| 2:M:704:ILE:HD11    | 2:M:711:ILE:HA   | 1.61                     | 0.80              |
| 2:P:588:MET:HE1     | 2:P:604:ILE:CD1  | 2.06                     | 0.80              |
| 1:C:577[A]:VAL:HG21 | 1:C:645:ILE:HG23 | 1.62                     | 0.80              |
| 1:D:539:ILE:CG2     | 1:D:540:GLY:N    | 2.44                     | 0.80              |
| 2:O:348:PRO:CG      | 2:O:475:LYS:CE   | 2.59                     | 0.80              |
| 2:O:490:ASP:CB      | 2:O:491:ARG:NH1  | 2.42                     | 0.80              |
| 2:O:350:PHE:HD2     | 2:O:385:GLY:HA3  | 1.42                     | 0.80              |
| 2:O:351:GLU:CB      | 2:O:426:ASN:HD21 | 1.95                     | 0.80              |
| 1:C:220:HIS:HD2     | 1:C:221:MET:O    | 1.65                     | 0.79              |
| 2:O:343:GLY:HA2     | 2:O:349:ALA:HB2  | 1.65                     | 0.79              |
| 2:O:421:GLY:HA3     | 2:O:425:ILE:O    | 1.82                     | 0.79              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 1:A:535:ALA:HB3     | 1:A:537:ILE:CD1  | 2.12                     | 0.79              |
| 1:D:466:LEU:HD22    | 1:D:595:TRP:CZ2  | 2.19                     | 0.78              |
| 2:N:490:ASP:O       | 2:N:493:ARG:HG3  | 1.84                     | 0.78              |
| 2:O:467:ILE:HD12    | 2:O:467:ILE:N    | 1.98                     | 0.78              |
| 2:O:351:GLU:HG2     | 2:O:423:ARG:N    | 1.99                     | 0.78              |
| 2:O:351:GLU:HB2     | 2:O:426:ASN:HD21 | 1.46                     | 0.78              |
| 2:O:381:LYS:O       | 2:O:383:PRO:HD3  | 1.84                     | 0.77              |
| 1:B:529:LYS:CB      | 10:B:1156:HOH:O  | 2.32                     | 0.77              |
| 2:M:320:LEU:HB3     | 2:M:321:PRO:HD2  | 1.66                     | 0.77              |
| 2:M:471:GLU:O       | 2:M:475:LYS:HB2  | 1.83                     | 0.77              |
| 2:P:361:ILE:HG13    | 2:P:464:GLN:HG2  | 1.67                     | 0.77              |
| 2:O:396:GLN:NE2     | 2:O:399:PHE:CD1  | 2.51                     | 0.77              |
| 2:O:480:VAL:HA      | 2:O:483:GLU:OE1  | 1.84                     | 0.77              |
| 5:C:863:GOL:H31     | 2:O:27:HIS:HE1   | 1.46                     | 0.77              |
| 2:M:7:ILE:HD13      | 2:M:245:ARG:HD2  | 1.64                     | 0.77              |
| 2:M:426:ASN:HD22    | 2:M:426:ASN:H    | 1.32                     | 0.77              |
| 2:O:363:ASP:OD1     | 2:O:462:ARG:HA   | 1.85                     | 0.77              |
| 1:B:529:LYS:HB3     | 10:B:1156:HOH:O  | 1.85                     | 0.76              |
| 1:D:577[A]:VAL:HG21 | 1:D:645:ILE:HG23 | 1.67                     | 0.76              |
| 1:C:283:HIS:CD2     | 1:C:317:CYS:HB2  | 2.21                     | 0.76              |
| 2:N:346:ARG:HB3     | 2:N:381:LYS:HD2  | 1.66                     | 0.76              |
| 2:O:649:ARG:HA      | 2:O:652:ILE:HD12 | 1.66                     | 0.76              |
| 2:O:723:LEU:C       | 2:O:723:LEU:CD2  | 2.59                     | 0.76              |
| 2:O:483:GLU:HG2     | 2:O:484:LYS:H    | 1.48                     | 0.76              |
| 2:P:359:SER:C       | 2:P:361:ILE:H    | 1.93                     | 0.76              |
| 1:C:614:ASP:H       | 5:C:863:GOL:H32  | 1.51                     | 0.76              |
| 1:B:35:GLU:OE1      | 1:B:421:PRO:HB3  | 1.86                     | 0.75              |
| 2:P:424:ASN:H       | 2:P:424:ASN:HD22 | 1.32                     | 0.75              |
| 1:A:284:ASN:HD22    | 1:A:286:LEU:H    | 1.34                     | 0.75              |
| 5:D:863:GOL:H2      | 2:P:27:HIS:CE1   | 2.21                     | 0.75              |
| 2:N:478:MET:O       | 2:N:482:ARG:HG3  | 1.85                     | 0.75              |
| 2:P:602:MET:HE2     | 2:P:647:ILE:HG21 | 1.68                     | 0.75              |
| 2:M:602:MET:HE3     | 2:M:647:ILE:CD1  | 2.15                     | 0.75              |
| 2:P:150:ASP:OD2     | 2:P:152:THR:CG2  | 2.35                     | 0.75              |
| 2:O:396:GLN:OE1     | 2:O:396:GLN:C    | 2.30                     | 0.75              |
| 2:N:187:ASP:HA      | 2:N:211:ASN:HD22 | 1.52                     | 0.75              |
| 2:N:602:MET:HE1     | 2:N:658:ILE:HG21 | 1.68                     | 0.74              |
| 2:O:476:GLU:C       | 2:O:476:GLU:OE1  | 2.30                     | 0.74              |
| 2:O:478:MET:O       | 2:O:481:ALA:HB3  | 1.88                     | 0.74              |
| 2:O:384:LEU:HD12    | 2:O:385:GLY:H    | 1.52                     | 0.74              |
| 2:O:484:LYS:O       | 2:O:485:TYR:C    | 2.30                     | 0.74              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 2:O:464:GLN:NE2     | 2:O:466:THR:HG23 | 2.02                     | 0.73              |
| 1:C:209:HIS:HD2     | 1:D:213:SER:CB   | 2.02                     | 0.73              |
| 1:C:60:LYS:O        | 1:C:64:GLU:HG3   | 1.87                     | 0.73              |
| 2:O:371:PRO:CD      | 2:O:469:THR:OG1  | 2.34                     | 0.73              |
| 2:O:351:GLU:O       | 2:O:352:LEU:HB3  | 1.88                     | 0.73              |
| 2:O:374:ASP:HB3     | 2:O:440:ARG:NE   | 2.03                     | 0.73              |
| 2:P:316:ILE:HG23    | 2:P:316:ILE:O    | 1.88                     | 0.73              |
| 1:A:577[B]:VAL:HG11 | 1:A:645:ILE:HG23 | 1.69                     | 0.72              |
| 2:M:406:ARG:NH1     | 2:M:409:ASP:OD2  | 2.20                     | 0.72              |
| 1:A:192:GLU:O       | 1:A:196:GLU:HG3  | 1.88                     | 0.72              |
| 2:O:480:VAL:HG12    | 2:O:481:ALA:N    | 2.02                     | 0.72              |
| 2:O:353:VAL:HG12    | 2:O:388:VAL:HB   | 1.72                     | 0.72              |
| 1:D:510:LEU:HD12    | 1:D:510:LEU:N    | 2.05                     | 0.72              |
| 2:O:491:ARG:NH1     | 2:O:491:ARG:H    | 1.88                     | 0.71              |
| 2:O:349:ALA:HB3     | 2:O:424:ASN:O    | 1.91                     | 0.71              |
| 2:O:351:GLU:HB3     | 2:O:423:ARG:CA   | 2.20                     | 0.71              |
| 2:O:347:THR:HG23    | 2:O:383:PRO:HG3  | 1.72                     | 0.71              |
| 2:O:626:MET:HB2     | 2:O:631:LEU:HD13 | 1.73                     | 0.71              |
| 2:O:355:THR:OG1     | 2:O:395:MET:HG3  | 1.91                     | 0.70              |
| 2:O:650:THR:HG22    | 2:O:650:THR:O    | 1.91                     | 0.70              |
| 2:O:157:ALA:HB3     | 2:O:183:LEU:HD22 | 1.71                     | 0.70              |
| 2:O:349:ALA:HB1     | 2:O:426:ASN:OD1  | 1.91                     | 0.70              |
| 2:O:557:ILE:CD1     | 2:O:565:LYS:HG3  | 2.17                     | 0.70              |
| 2:O:666:ARG:NH2     | 2:O:725:MET:CE   | 2.54                     | 0.70              |
| 2:P:505:SER:HB3     | 2:P:570:TYR:CE2  | 2.26                     | 0.70              |
| 2:P:670:MET:HE3     | 2:P:675:LYS:HG2  | 1.74                     | 0.70              |
| 2:O:384:LEU:C       | 2:O:474:VAL:HG21 | 2.17                     | 0.70              |
| 2:O:343:GLY:HA3     | 2:O:349:ALA:HB2  | 1.72                     | 0.70              |
| 2:O:396:GLN:HG3     | 2:O:399:PHE:HD1  | 1.56                     | 0.70              |
| 1:D:299:GLU:OE2     | 1:D:299:GLU:HA   | 1.91                     | 0.69              |
| 2:O:509:CYS:HB3     | 8:O:953:ACT:H3   | 1.74                     | 0.69              |
| 2:O:666:ARG:CZ      | 2:O:725:MET:CE   | 2.71                     | 0.69              |
| 2:O:478:MET:O       | 2:O:481:ALA:N    | 2.25                     | 0.69              |
| 2:O:124:ASP:C       | 2:O:125:GLU:HG2  | 2.18                     | 0.69              |
| 2:O:480:VAL:O       | 2:O:481:ALA:C    | 2.34                     | 0.69              |
| 2:N:384:LEU:HD11    | 2:N:467:ILE:CG2  | 2.22                     | 0.69              |
| 2:O:396:GLN:HE22    | 2:O:398:ASP:HB2  | 1.57                     | 0.69              |
| 2:O:374:ASP:HB3     | 2:O:440:ARG:HE   | 1.58                     | 0.69              |
| 2:O:427:TRP:O       | 2:O:428:LEU:HD22 | 1.93                     | 0.69              |
| 2:O:728:ILE:O       | 2:O:728:ILE:HD12 | 1.92                     | 0.68              |
| 2:O:473:LYS:C       | 2:O:476:GLU:H    | 2.02                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:C:615:LEU:C      | 1:C:615:LEU:HD23 | 2.18                     | 0.68              |
| 2:O:108:TYR:O      | 2:O:112:ILE:HG13 | 1.93                     | 0.68              |
| 2:O:524:ARG:O      | 2:O:524:ARG:HG3  | 1.93                     | 0.68              |
| 2:M:588:MET:HE1    | 2:M:604:ILE:HG23 | 1.76                     | 0.68              |
| 1:C:601:PRO:HD3    | 1:C:652:ARG:NH2  | 2.09                     | 0.68              |
| 2:O:685:ARG:O      | 2:O:688:GLU:CB   | 2.33                     | 0.68              |
| 2:P:486:LYS:HA     | 2:P:489:ASP:HB2  | 1.76                     | 0.67              |
| 2:P:602:MET:HE3    | 2:P:647:ILE:HG21 | 1.76                     | 0.67              |
| 2:O:333:ILE:HD12   | 2:O:429:ARG:HB3  | 1.76                     | 0.67              |
| 2:P:149:VAL:HG11   | 8:P:953:ACT:H3   | 1.76                     | 0.67              |
| 2:N:408:HIS:HD2    | 2:N:419:HIS:ND1  | 1.91                     | 0.67              |
| 2:O:486:LYS:O      | 2:O:489:ASP:HB3  | 1.93                     | 0.67              |
| 1:D:614:ASP:N      | 5:D:863:GOL:H11  | 2.09                     | 0.67              |
| 2:M:439:PHE:CE1    | 2:M:443:ASN:HB2  | 2.29                     | 0.67              |
| 2:O:162:ARG:HG3    | 2:O:188:GLU:HB2  | 1.77                     | 0.67              |
| 2:M:377:PRO:O      | 2:M:380:SER:HB3  | 1.94                     | 0.67              |
| 2:O:348:PRO:HG2    | 2:O:475:LYS:CE   | 2.25                     | 0.67              |
| 2:O:605:LEU:HB3    | 2:O:608:CYS:HB2  | 1.77                     | 0.67              |
| 1:A:655:LYS:NZ     | 1:A:674:TYR:O    | 2.28                     | 0.67              |
| 1:D:68:CYS:HB2     | 1:D:97:ILE:CG2   | 2.24                     | 0.67              |
| 2:O:360:GLU:O      | 2:O:361:ILE:HB   | 1.94                     | 0.67              |
| 2:O:365:LYS:HG2    | 2:O:464:GLN:CG   | 2.24                     | 0.66              |
| 2:M:23:ARG:NH1     | 10:M:793:HOH:O   | 2.27                     | 0.66              |
| 2:P:80:PRO:HB2     | 2:P:81:PRO:HD3   | 1.76                     | 0.66              |
| 1:C:209:HIS:HD2    | 1:D:213:SER:OG   | 1.78                     | 0.66              |
| 2:M:424:ASN:HD22   | 2:M:424:ASN:H    | 1.43                     | 0.66              |
| 2:P:444:TYR:O      | 2:P:448:LEU:CD2  | 2.39                     | 0.66              |
| 2:O:691:LEU:HD21   | 2:O:721:PRO:HG2  | 1.76                     | 0.66              |
| 2:O:340:VAL:HG21   | 2:O:382:LEU:HB2  | 1.78                     | 0.66              |
| 2:O:351:GLU:CB     | 2:O:426:ASN:ND2  | 2.56                     | 0.66              |
| 2:P:341:GLU:CD     | 2:P:427:TRP:HE1  | 2.04                     | 0.66              |
| 1:C:213:SER:CB     | 1:D:209:HIS:HD2  | 2.08                     | 0.65              |
| 1:D:149[A]:ARG:HD3 | 10:D:1162:HOH:O  | 1.96                     | 0.65              |
| 1:D:284:ASN:HD22   | 1:D:286:LEU:H    | 1.42                     | 0.65              |
| 2:M:426:ASN:HD22   | 2:M:426:ASN:N    | 1.94                     | 0.65              |
| 2:O:230:GLY:HA3    | 2:O:243:TYR:CE2  | 2.32                     | 0.65              |
| 2:O:670:MET:HE2    | 2:O:674:LEU:HG   | 1.77                     | 0.65              |
| 2:O:342:MET:O      | 2:O:427:TRP:HA   | 1.95                     | 0.65              |
| 2:O:469:THR:O      | 2:O:470:ASP:HB2  | 1.95                     | 0.65              |
| 1:A:515:ASN:HD22   | 1:A:518:THR:CG2  | 2.09                     | 0.65              |
| 2:M:602:MET:HE1    | 2:M:657:PHE:HE2  | 1.62                     | 0.65              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 2:O:224:ARG:O       | 2:O:228:MET:HB2  | 1.95                     | 0.65              |
| 2:O:715:LEU:HD22    | 2:O:720:HIS:CD2  | 2.29                     | 0.65              |
| 2:O:3:ASP:O         | 2:O:6:LYS:HG2    | 1.97                     | 0.65              |
| 2:O:422:GLN:N       | 2:O:422:GLN:OE1  | 2.30                     | 0.65              |
| 2:O:384:LEU:HD13    | 2:O:468:PHE:O    | 1.97                     | 0.65              |
| 2:O:685:ARG:HB3     | 2:O:685:ARG:HH11 | 1.62                     | 0.65              |
| 1:C:98:VAL:O        | 1:C:102:VAL:HG12 | 1.97                     | 0.64              |
| 1:C:260:GLN:HG2     | 10:C:1398:HOH:O  | 1.97                     | 0.64              |
| 2:O:407:ILE:HG23    | 2:O:411:ILE:HD13 | 1.77                     | 0.64              |
| 2:O:428:LEU:HD22    | 2:O:428:LEU:N    | 2.12                     | 0.64              |
| 2:M:655:LYS:HE3     | 10:M:901:HOH:O   | 1.96                     | 0.64              |
| 2:O:469:THR:O       | 2:O:470:ASP:CB   | 2.45                     | 0.64              |
| 1:D:515:ASN:HA      | 1:D:518:THR:HG22 | 1.80                     | 0.64              |
| 1:B:283:HIS:CD2     | 1:B:317:CYS:HB2  | 2.32                     | 0.64              |
| 1:D:195:LYS:O       | 1:D:199:ARG:HG3  | 1.97                     | 0.64              |
| 2:N:335:LYS:CD      | 2:N:335:LYS:N    | 2.40                     | 0.64              |
| 1:C:587:LYS:O       | 1:C:591:ILE:HG13 | 1.98                     | 0.64              |
| 1:C:601:PRO:HD3     | 1:C:652:ARG:CZ   | 2.28                     | 0.64              |
| 2:N:246[B]:ARG:HH12 | 2:N:247:ARG:HH11 | 1.43                     | 0.64              |
| 2:N:443:ASN:ND2     | 2:N:446:GLU:OE1  | 2.30                     | 0.64              |
| 2:M:314:THR:O       | 2:M:315:LYS:C    | 2.39                     | 0.64              |
| 2:M:721:PRO:O       | 2:M:725:MET:HG3  | 1.97                     | 0.64              |
| 2:O:352:LEU:CD1     | 2:O:484:LYS:HG3  | 2.28                     | 0.63              |
| 2:O:508:LEU:HD23    | 3:O:900:SF4:S1   | 2.38                     | 0.63              |
| 2:N:150:ASP:OD2     | 2:N:152:THR:HG22 | 1.99                     | 0.63              |
| 2:O:482:ARG:CA      | 2:O:482:ARG:NE   | 2.59                     | 0.63              |
| 2:M:344:GLY:O       | 2:M:346:ARG:NH1  | 2.32                     | 0.63              |
| 2:O:447:ILE:O       | 2:O:451:LYS:HB2  | 1.98                     | 0.63              |
| 1:D:283:HIS:CD2     | 1:D:317:CYS:HB2  | 2.34                     | 0.63              |
| 2:N:492:MET:HG2     | 10:N:1002:HOH:O  | 1.97                     | 0.63              |
| 2:N:540:TYR:CD1     | 2:N:550:PRO:HD3  | 2.34                     | 0.63              |
| 2:N:609:ASN:ND2     | 2:N:666:ARG:HH12 | 1.97                     | 0.62              |
| 2:O:169:LEU:HD13    | 2:O:193:LEU:CD2  | 2.29                     | 0.62              |
| 1:A:283:HIS:CD2     | 1:A:317:CYS:HB2  | 2.34                     | 0.62              |
| 1:C:294:ALA:O       | 1:C:298:MET:HG2  | 1.99                     | 0.62              |
| 1:C:587:LYS:H       | 1:D:220:HIS:HE1  | 1.48                     | 0.62              |
| 2:M:568:ASN:HD21    | 2:M:581:GLN:HE21 | 1.48                     | 0.62              |
| 1:C:615:LEU:HD23    | 1:C:615:LEU:O    | 2.00                     | 0.62              |
| 2:N:315:LYS:N       | 2:N:315:LYS:CE   | 2.63                     | 0.62              |
| 2:O:64:VAL:HB       | 2:O:223:LEU:HD12 | 1.81                     | 0.62              |
| 1:C:23:LYS:HE3      | 10:C:931:HOH:O   | 1.98                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:404:GLU:OE1  | 2:O:423:ARG:NE   | 2.34                     | 0.61              |
| 2:O:564:TRP:HB2  | 2:O:567:VAL:HB   | 1.82                     | 0.61              |
| 2:P:666:ARG:HD2  | 2:P:728:ILE:HD12 | 1.81                     | 0.61              |
| 2:N:316:ILE:O    | 2:N:317:LYS:C    | 2.42                     | 0.61              |
| 2:N:354:ARG:HD2  | 2:N:389:ASP:OD2  | 2.00                     | 0.61              |
| 1:B:200:THR:OG1  | 1:B:201:HIS:HD2  | 1.84                     | 0.61              |
| 2:O:490:ASP:O    | 2:O:492:MET:N    | 2.33                     | 0.61              |
| 2:P:583:CYS:CB   | 2:P:586:THR:HG22 | 2.30                     | 0.61              |
| 1:A:114:CYS:HB2  | 10:A:1315:HOH:O  | 2.00                     | 0.61              |
| 2:O:95:ASN:ND2   | 2:O:98:ASN:H     | 1.98                     | 0.61              |
| 2:M:348:PRO:HD2  | 2:M:383:PRO:HB3  | 1.82                     | 0.61              |
| 2:P:66:ARG:O     | 2:P:70:GLY:HA2   | 2.01                     | 0.61              |
| 2:P:316:ILE:O    | 2:P:316:ILE:CG2  | 2.49                     | 0.61              |
| 1:C:220:HIS:HE1  | 1:D:587:LYS:H    | 1.49                     | 0.61              |
| 2:M:704:ILE:HD13 | 2:M:714:TYR:CB   | 2.30                     | 0.61              |
| 2:O:385:GLY:N    | 2:O:474:VAL:HG21 | 2.16                     | 0.61              |
| 2:O:420:THR:O    | 2:O:426:ASN:HA   | 2.00                     | 0.61              |
| 2:P:602:MET:HE2  | 2:P:647:ILE:HD13 | 1.81                     | 0.61              |
| 2:P:289:PRO:O    | 2:P:290:ASP:HB2  | 2.00                     | 0.61              |
| 1:A:122:HIS:HD2  | 10:A:902:HOH:O   | 1.83                     | 0.61              |
| 2:O:478:MET:O    | 2:O:482:ARG:N    | 2.33                     | 0.61              |
| 2:P:166:SER:HB2  | 2:P:196:GLU:OE2  | 1.99                     | 0.61              |
| 2:P:359:SER:O    | 2:P:361:ILE:N    | 2.34                     | 0.61              |
| 2:M:342:MET:SD   | 2:M:342:MET:N    | 2.73                     | 0.61              |
| 2:O:360:GLU:O    | 2:O:361:ILE:CB   | 2.49                     | 0.61              |
| 2:O:351:GLU:CB   | 2:O:423:ARG:N    | 2.62                     | 0.60              |
| 1:B:515:ASN:HA   | 1:B:518:THR:HG23 | 1.84                     | 0.60              |
| 2:O:420:THR:HG1  | 2:O:427:TRP:HE3  | 0.65                     | 0.60              |
| 2:M:457:PRO:O    | 2:M:458:ALA:HB3  | 2.00                     | 0.60              |
| 2:O:346:ARG:HH22 | 2:O:381:LYS:NZ   | 2.00                     | 0.60              |
| 2:P:726:ASP:OD1  | 2:P:726:ASP:N    | 2.33                     | 0.60              |
| 2:O:557:ILE:HD11 | 2:O:565:LYS:CG   | 2.22                     | 0.60              |
| 2:P:602:MET:HG3  | 2:P:647:ILE:HD13 | 1.83                     | 0.60              |
| 1:A:220:HIS:HD2  | 1:A:221:MET:O    | 1.84                     | 0.60              |
| 2:O:351:GLU:CB   | 2:O:423:ARG:H    | 2.15                     | 0.60              |
| 1:D:399:THR:O    | 1:D:403:MET:HG3  | 2.02                     | 0.60              |
| 2:O:388:VAL:HG13 | 2:O:465:VAL:HG22 | 1.84                     | 0.60              |
| 2:P:428:LEU:N    | 2:P:428:LEU:HD12 | 2.16                     | 0.60              |
| 2:O:426:ASN:OD1  | 2:O:426:ASN:N    | 2.34                     | 0.59              |
| 2:P:199:LYS:HE2  | 2:P:415:GLU:OE2  | 2.03                     | 0.59              |
| 2:N:560:ILE:O    | 2:N:660:ALA:HB2  | 2.02                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 2:M:167:LYS:HD3     | 2:M:196:GLU:OE1  | 2.01                     | 0.59              |
| 2:O:347:THR:CG2     | 2:O:383:PRO:HG3  | 2.32                     | 0.59              |
| 2:O:712:LEU:HB3     | 2:O:713:PRO:CD   | 2.31                     | 0.59              |
| 1:D:510:LEU:HD12    | 1:D:510:LEU:H    | 1.65                     | 0.59              |
| 1:A:535:ALA:HB3     | 1:A:537:ILE:HD12 | 1.85                     | 0.59              |
| 2:P:238:GLU:HG2     | 10:P:735:HOH:O   | 2.01                     | 0.59              |
| 2:O:169:LEU:HD13    | 2:O:193:LEU:HD21 | 1.85                     | 0.59              |
| 1:A:284:ASN:HD21    | 1:A:286:LEU:HG   | 1.68                     | 0.59              |
| 1:D:149[A]:ARG:NH2  | 1:D:250:ASP:OD2  | 2.36                     | 0.59              |
| 2:P:340:VAL:HG21    | 2:P:376:ILE:HD11 | 1.85                     | 0.59              |
| 2:N:384:LEU:HD11    | 2:N:467:ILE:HG23 | 1.85                     | 0.58              |
| 2:O:467:ILE:N       | 2:O:467:ILE:CD1  | 2.65                     | 0.58              |
| 1:B:305:ALA:CB      | 1:B:409:LYS:HE3  | 2.34                     | 0.58              |
| 2:O:71:GLU:HG3      | 2:O:82:ILE:HD11  | 1.85                     | 0.58              |
| 2:O:470:ASP:O       | 2:O:474:VAL:HG12 | 2.02                     | 0.58              |
| 1:A:515:ASN:HD22    | 1:A:518:THR:HG21 | 1.68                     | 0.58              |
| 2:P:488:ARG:C       | 2:P:490:ASP:H    | 2.12                     | 0.58              |
| 1:A:316:CYS:H       | 1:A:503:GLN:HE22 | 1.52                     | 0.58              |
| 1:C:112:ALA:HA      | 1:D:217:ASN:HD22 | 1.69                     | 0.58              |
| 2:N:150:ASP:OD2     | 2:N:152:THR:CG2  | 2.52                     | 0.58              |
| 1:B:615:LEU:HD23    | 1:B:615:LEU:C    | 2.29                     | 0.58              |
| 2:P:457:PRO:O       | 2:P:458:ALA:HB2  | 2.03                     | 0.58              |
| 1:C:456:ILE:HD13    | 1:C:463:GLY:HA2  | 1.86                     | 0.58              |
| 2:O:95:ASN:C        | 2:O:95:ASN:HD22  | 2.11                     | 0.58              |
| 1:B:661[A]:GLU:HG3  | 1:B:665:ARG:HH21 | 1.66                     | 0.58              |
| 2:O:367:GLU:OE1     | 2:O:369:ILE:HG12 | 2.04                     | 0.58              |
| 2:O:665:ALA:O       | 2:O:722:ALA:HB2  | 2.03                     | 0.58              |
| 1:A:220:HIS:HE1     | 1:B:587:LYS:H    | 1.52                     | 0.57              |
| 1:D:466:LEU:HD22    | 1:D:595:TRP:HZ2  | 1.66                     | 0.57              |
| 2:O:355:THR:HG21    | 2:O:395:MET:HB3  | 1.86                     | 0.57              |
| 2:O:396:GLN:OE1     | 2:O:397:ALA:N    | 2.37                     | 0.57              |
| 1:A:177:LEU:HB2     | 1:A:180:GLU:CD   | 2.29                     | 0.57              |
| 1:C:577[B]:VAL:HG23 | 1:C:649:LEU:CD2  | 2.35                     | 0.57              |
| 1:D:577[A]:VAL:HG21 | 1:D:645:ILE:CG2  | 2.34                     | 0.57              |
| 2:P:318:LEU:HD13    | 2:P:320:LEU:HD11 | 1.85                     | 0.57              |
| 1:C:368:HIS:HE1     | 1:C:416:ARG:CB   | 2.18                     | 0.57              |
| 2:O:384:LEU:CD1     | 2:O:468:PHE:O    | 2.53                     | 0.57              |
| 2:O:478:MET:C       | 2:O:480:VAL:N    | 2.62                     | 0.57              |
| 2:O:613:ILE:HD12    | 2:O:670:MET:HE3  | 1.85                     | 0.57              |
| 2:O:464:GLN:HE22    | 2:O:466:THR:HG23 | 1.67                     | 0.57              |
| 2:O:6:LYS:O         | 2:O:9:GLU:HB2    | 2.04                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 2:P:568:ASN:ND2     | 2:P:581:GLN:HB2  | 2.19                     | 0.57              |
| 2:N:315:LYS:CE      | 2:N:315:LYS:CA   | 2.78                     | 0.57              |
| 2:M:602:MET:HE1     | 2:M:647:ILE:HD13 | 1.80                     | 0.57              |
| 2:O:685:ARG:HB3     | 2:O:685:ARG:CZ   | 2.31                     | 0.57              |
| 2:P:359:SER:C       | 2:P:361:ILE:N    | 2.61                     | 0.57              |
| 1:C:138:LYS:HG3     | 1:C:255:LEU:O    | 2.05                     | 0.57              |
| 2:P:602:MET:HE3     | 2:P:647:ILE:CG2  | 2.34                     | 0.57              |
| 1:B:267:ASN:O       | 1:B:270:VAL:HG22 | 2.05                     | 0.56              |
| 2:M:727:PRO:HG3     | 2:O:367:GLU:HG2  | 1.86                     | 0.56              |
| 2:O:477:TYR:O       | 2:O:480:VAL:CB   | 2.41                     | 0.56              |
| 2:O:479:GLU:HA      | 2:O:482:ARG:HB2  | 1.87                     | 0.56              |
| 1:A:399:THR:HG22    | 1:A:403:MET:HE3  | 1.86                     | 0.56              |
| 1:D:128:ALA:HA      | 1:D:160:LEU:HD22 | 1.87                     | 0.56              |
| 2:O:157:ALA:HB3     | 2:O:183:LEU:HD23 | 1.87                     | 0.56              |
| 1:B:368:HIS:NE2     | 1:B:416:ARG:HD2  | 2.20                     | 0.56              |
| 2:O:232:VAL:CG1     | 2:O:239:GLU:HB3  | 2.35                     | 0.56              |
| 2:O:623:PRO:HA      | 2:O:707:THR:HA   | 1.86                     | 0.56              |
| 1:C:357:MET:O       | 1:C:360:ILE:HG12 | 2.05                     | 0.56              |
| 1:D:469:GLY:C       | 4:D:800:XCC:S1   | 2.88                     | 0.56              |
| 2:O:340:VAL:HG23    | 2:O:382:LEU:H    | 1.70                     | 0.56              |
| 1:B:577[A]:VAL:HG21 | 1:B:645:ILE:HG23 | 1.88                     | 0.56              |
| 2:P:150:ASP:CG      | 2:P:152:THR:HG22 | 2.30                     | 0.56              |
| 2:N:246[B]:ARG:NH1  | 2:N:247:ARG:NH1  | 2.41                     | 0.56              |
| 2:N:369:ILE:HD12    | 2:N:468:PHE:CE2  | 2.41                     | 0.56              |
| 2:O:483:GLU:HG3     | 2:O:484:LYS:H    | 1.44                     | 0.56              |
| 1:A:335:ALA:H       | 1:A:471:ASN:HD22 | 1.52                     | 0.56              |
| 1:B:2:PRO:N         | 1:B:625:SER:HG   | 2.03                     | 0.56              |
| 2:O:248:ILE:O       | 2:O:309:ARG:NH2  | 2.37                     | 0.56              |
| 1:A:126:GLU:OE1     | 1:A:390:THR:OG1  | 2.21                     | 0.55              |
| 2:O:649:ARG:HA      | 2:O:652:ILE:CD1  | 2.34                     | 0.55              |
| 1:D:149[B]:ARG:NH2  | 1:D:250:ASP:OD2  | 2.38                     | 0.55              |
| 2:N:315:LYS:HE2     | 2:N:315:LYS:CA   | 2.36                     | 0.55              |
| 1:C:213:SER:OG      | 1:D:209:HIS:HD2  | 1.89                     | 0.55              |
| 1:D:220:HIS:HD2     | 1:D:221:MET:O    | 1.88                     | 0.55              |
| 2:M:354:ARG:HH21    | 2:M:480:VAL:HG11 | 1.71                     | 0.55              |
| 2:M:408:HIS:HD2     | 2:M:419:HIS:ND1  | 2.05                     | 0.55              |
| 2:N:342:MET:SD      | 2:N:342:MET:N    | 2.79                     | 0.55              |
| 2:O:666:ARG:CZ      | 2:O:725:MET:HE2  | 2.37                     | 0.55              |
| 2:O:685:ARG:C       | 2:O:688:GLU:HB3  | 2.27                     | 0.55              |
| 2:O:333:ILE:HD12    | 2:O:429:ARG:CB   | 2.36                     | 0.55              |
| 2:O:473:LYS:O       | 2:O:476:GLU:HB3  | 2.07                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:O:602:MET:HE1   | 2:O:645:MET:HE2    | 1.89                     | 0.55              |
| 2:O:712:LEU:HB3   | 2:O:713:PRO:HD3    | 1.88                     | 0.55              |
| 1:C:217:ASN:HD22  | 1:D:112:ALA:HA     | 1.71                     | 0.55              |
| 2:N:482:ARG:O     | 2:N:486[A]:LYS:HG3 | 2.05                     | 0.55              |
| 2:O:398:ASP:C     | 2:O:400:GLU:H      | 2.15                     | 0.55              |
| 1:D:144:LYS:O     | 1:D:148:ARG:HG3    | 2.06                     | 0.55              |
| 2:O:340:VAL:CG2   | 2:O:382:LEU:H      | 2.19                     | 0.55              |
| 2:O:430:VAL:HG12  | 2:O:431:SER:N      | 2.21                     | 0.55              |
| 2:P:424:ASN:H     | 2:P:424:ASN:ND2    | 2.01                     | 0.55              |
| 2:O:396:GLN:CG    | 2:O:399:PHE:CD1    | 2.90                     | 0.55              |
| 2:P:602:MET:CE    | 2:P:645:MET:HE3    | 2.38                     | 0.54              |
| 1:C:614:ASP:H     | 5:C:863:GOL:C3     | 2.18                     | 0.54              |
| 2:N:442:LYS:HB2   | 10:N:1326:HOH:O    | 2.06                     | 0.54              |
| 1:C:68:CYS:HB2    | 1:C:97:ILE:HG23    | 1.90                     | 0.54              |
| 2:N:721:PRO:O     | 2:N:725:MET:HG3    | 2.07                     | 0.54              |
| 2:O:721:PRO:O     | 2:O:725:MET:HB2    | 2.07                     | 0.54              |
| 2:P:424:ASN:HD22  | 2:P:424:ASN:N      | 1.99                     | 0.54              |
| 1:B:539:ILE:HG13  | 1:B:540:GLY:H      | 1.72                     | 0.54              |
| 1:A:213:SER:OG    | 1:B:209:HIS:HD2    | 1.90                     | 0.54              |
| 1:B:35:GLU:OE2    | 1:B:423:ILE:HD11   | 2.07                     | 0.54              |
| 2:M:602:MET:HE1   | 2:M:657:PHE:CE2    | 2.43                     | 0.54              |
| 2:P:522:PRO:HD3   | 2:P:533:TRP:CD1    | 2.43                     | 0.54              |
| 2:M:117[B]:ARG:CZ | 2:M:127:LEU:HD23   | 2.37                     | 0.54              |
| 2:O:720:HIS:ND1   | 2:O:721:PRO:HD2    | 2.22                     | 0.54              |
| 1:C:129:GLU:OE2   | 1:C:164:GLN:NE2    | 2.40                     | 0.54              |
| 2:O:500:VAL:HG22  | 2:O:502:THR:H      | 1.73                     | 0.54              |
| 2:P:383:PRO:HB2   | 2:P:474:VAL:HG21   | 1.90                     | 0.54              |
| 1:C:182:GLU:HG2   | 1:C:204:VAL:HG11   | 1.88                     | 0.54              |
| 2:O:342:MET:SD    | 2:O:428:LEU:HB2    | 2.48                     | 0.54              |
| 2:O:396:GLN:CG    | 2:O:399:PHE:HD1    | 2.21                     | 0.54              |
| 2:O:481:ALA:O     | 2:O:482:ARG:C      | 2.51                     | 0.54              |
| 2:M:490:ASP:HA    | 2:M:493:ARG:NH1    | 2.23                     | 0.53              |
| 2:O:421:GLY:C     | 2:O:422:GLN:OE1    | 2.50                     | 0.53              |
| 1:B:28:THR:HG21   | 1:B:33:VAL:HG12    | 1.91                     | 0.53              |
| 1:C:408:PHE:O     | 1:C:411:ARG:HB3    | 2.07                     | 0.53              |
| 1:D:313:VAL:HG21  | 1:D:331:VAL:HG13   | 1.90                     | 0.53              |
| 2:O:396:GLN:C     | 2:O:396:GLN:CD     | 2.76                     | 0.53              |
| 1:B:201:HIS:HE1   | 2:N:35:TYR:OH      | 1.91                     | 0.53              |
| 1:B:444:ASN:HB3   | 1:B:451:VAL:HG23   | 1.91                     | 0.53              |
| 1:B:529:LYS:HB2   | 10:B:1156:HOH:O    | 2.01                     | 0.53              |
| 1:C:214:GLU:O     | 1:C:217:ASN:HB3    | 2.08                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 2:O:565:LYS:O       | 2:O:569:ASP:CG   | 2.51                     | 0.53              |
| 1:A:217:ASN:HD22    | 1:B:112:ALA:HA   | 1.74                     | 0.53              |
| 2:O:351:GLU:HB3     | 2:O:426:ASN:HD21 | 1.70                     | 0.53              |
| 1:A:201:HIS:CE1     | 2:M:35:TYR:OH    | 2.61                     | 0.53              |
| 1:B:656:LEU:HD22    | 1:B:660:LYS:HD2  | 1.89                     | 0.53              |
| 2:O:478:MET:O       | 2:O:481:ALA:CB   | 2.54                     | 0.53              |
| 1:D:614:ASP:H       | 5:D:863:GOL:H11  | 1.72                     | 0.53              |
| 2:N:400:GLU:HB3     | 2:N:488:ARG:NH2  | 2.24                     | 0.53              |
| 2:O:424:ASN:ND2     | 2:O:485:TYR:CE1  | 2.76                     | 0.53              |
| 1:B:220:HIS:HD2     | 1:B:221:MET:O    | 1.92                     | 0.52              |
| 1:C:577[B]:VAL:HG23 | 1:C:649:LEU:HD23 | 1.90                     | 0.52              |
| 2:O:483:GLU:O       | 2:O:486:LYS:CB   | 2.47                     | 0.52              |
| 2:P:408:HIS:HD2     | 2:P:419:HIS:ND1  | 2.07                     | 0.52              |
| 1:A:601:PRO:HD3     | 1:A:652:ARG:CZ   | 2.39                     | 0.52              |
| 1:D:587:LYS:HE3     | 4:D:800:XCC:S4   | 2.49                     | 0.52              |
| 2:N:587:LEU:HD22    | 2:N:602:MET:HE2  | 1.91                     | 0.52              |
| 1:A:209:HIS:HD2     | 1:B:213:SER:OG   | 1.92                     | 0.52              |
| 2:N:350:PHE:CD1     | 2:N:350:PHE:C    | 2.87                     | 0.52              |
| 2:O:351:GLU:HB3     | 2:O:423:ARG:HA   | 1.91                     | 0.52              |
| 2:O:424:ASN:CG      | 2:O:485:TYR:HE1  | 2.16                     | 0.52              |
| 2:O:666:ARG:CZ      | 2:O:725:MET:HE1  | 2.40                     | 0.52              |
| 1:A:535:ALA:CB      | 1:A:537:ILE:CD1  | 2.87                     | 0.52              |
| 2:O:316:ILE:HG13    | 2:O:454:GLU:HG3  | 1.92                     | 0.52              |
| 2:O:612:MET:HB3     | 2:O:669:TRP:HB3  | 1.90                     | 0.52              |
| 2:P:583:CYS:HB2     | 2:P:586:THR:HG22 | 1.92                     | 0.52              |
| 1:C:655:LYS:NZ      | 1:C:674:TYR:O    | 2.33                     | 0.52              |
| 2:O:602:MET:CE      | 2:O:645:MET:HE2  | 2.40                     | 0.52              |
| 2:M:478:MET:O       | 2:M:478:MET:HG3  | 2.09                     | 0.52              |
| 2:N:583:CYS:HB2     | 2:N:586:THR:HG22 | 1.90                     | 0.52              |
| 1:D:24:ASN:O        | 1:D:27:ARG:HG2   | 2.08                     | 0.52              |
| 2:O:488:ARG:HG3     | 2:O:488:ARG:NH1  | 2.24                     | 0.52              |
| 2:M:272:THR:HG22    | 2:M:272:THR:O    | 2.10                     | 0.52              |
| 2:O:367:GLU:OE2     | 2:O:369:ILE:CD1  | 2.53                     | 0.52              |
| 2:O:467:ILE:HG22    | 2:O:468:PHE:N    | 2.25                     | 0.52              |
| 2:P:369:ILE:HD13    | 2:P:473:LYS:HD2  | 1.92                     | 0.52              |
| 2:P:505:SER:HB3     | 2:P:570:TYR:HE2  | 1.74                     | 0.52              |
| 1:D:238:ALA:O       | 1:D:241:ASP:HB3  | 2.10                     | 0.51              |
| 2:O:122:LYS:HB2     | 2:O:125:GLU:HG3  | 1.91                     | 0.51              |
| 2:O:367:GLU:HB3     | 2:O:466:THR:HG22 | 1.91                     | 0.51              |
| 2:O:506:CYS:HB3     | 3:O:900:SF4:S4   | 2.51                     | 0.51              |
| 2:P:583:CYS:SG      | 2:P:589:GLU:HG2  | 2.51                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:426:ASN:H    | 2:M:426:ASN:ND2  | 2.05                     | 0.51              |
| 2:N:187:ASP:HA   | 2:N:211:ASN:ND2  | 2.23                     | 0.51              |
| 2:O:698:LYS:HG2  | 2:O:718:LYS:HD2  | 1.92                     | 0.51              |
| 2:P:583:CYS:HB3  | 2:P:586:THR:HG22 | 1.92                     | 0.51              |
| 1:C:221:MET:HE2  | 1:D:584:MET:HE2  | 1.91                     | 0.51              |
| 1:D:18:ARG:NE    | 1:D:636:MET:HE3  | 2.25                     | 0.51              |
| 2:M:351:GLU:OE2  | 2:M:422:GLN:HA   | 2.11                     | 0.51              |
| 2:O:66:ARG:NH1   | 2:O:234:PRO:HG2  | 2.25                     | 0.51              |
| 2:O:478:MET:C    | 2:O:480:VAL:H    | 2.18                     | 0.51              |
| 2:P:425:ILE:HG22 | 2:P:425:ILE:O    | 2.10                     | 0.51              |
| 1:B:153:GLU:OE1  | 1:B:155:GLU:CD   | 2.54                     | 0.51              |
| 1:D:364:ALA:HB1  | 1:D:369:THR:HB   | 1.92                     | 0.51              |
| 2:O:166:SER:HB2  | 2:O:196:GLU:CG   | 2.41                     | 0.51              |
| 2:O:626:MET:SD   | 2:O:631:LEU:HD12 | 2.51                     | 0.51              |
| 2:O:684:ARG:NH1  | 2:O:685:ARG:HG2  | 2.25                     | 0.51              |
| 2:P:422:GLN:HE21 | 2:P:422:GLN:N    | 2.08                     | 0.51              |
| 2:P:585:TYR:CE2  | 2:P:656:LYS:HD2  | 2.45                     | 0.51              |
| 1:C:281:HIS:HB3  | 1:C:351:VAL:HG12 | 1.92                     | 0.51              |
| 2:N:266:ALA:O    | 2:N:269:ALA:HB3  | 2.09                     | 0.51              |
| 1:D:118:ASN:C    | 1:D:118:ASN:HD22 | 2.19                     | 0.51              |
| 1:D:284:ASN:ND2  | 1:D:286:LEU:H    | 2.08                     | 0.51              |
| 2:N:596:GLY:HA2  | 2:N:598:PHE:CE2  | 2.45                     | 0.51              |
| 2:O:113:ILE:O    | 2:O:117:ARG:HG3  | 2.10                     | 0.51              |
| 2:O:473:LYS:O    | 2:O:476:GLU:CB   | 2.58                     | 0.51              |
| 2:P:684:ARG:O    | 2:P:688:GLU:HG3  | 2.11                     | 0.51              |
| 1:C:209:HIS:CD2  | 1:D:213:SER:CB   | 2.89                     | 0.51              |
| 2:M:372:ASP:H    | 2:M:375:GLN:NE2  | 2.09                     | 0.51              |
| 2:O:384:LEU:HD12 | 2:O:385:GLY:N    | 2.25                     | 0.51              |
| 2:O:482:ARG:CZ   | 2:O:482:ARG:N    | 2.74                     | 0.51              |
| 2:O:484:LYS:O    | 2:O:485:TYR:O    | 2.29                     | 0.51              |
| 2:O:490:ASP:CB   | 2:O:491:ARG:HH11 | 2.24                     | 0.51              |
| 2:P:358:GLU:HG3  | 2:P:391:TYR:CE2  | 2.46                     | 0.51              |
| 2:O:160:LEU:HD13 | 2:O:215:ILE:HD13 | 1.93                     | 0.50              |
| 2:O:365:LYS:CG   | 2:O:464:GLN:HG3  | 2.35                     | 0.50              |
| 2:O:435:VAL:C    | 2:O:437:LYS:H    | 2.19                     | 0.50              |
| 1:A:584:MET:HE3  | 1:B:73:ALA:CB    | 2.40                     | 0.50              |
| 2:N:7:ILE:HD13   | 2:N:245:ARG:HD2  | 1.94                     | 0.50              |
| 2:N:419:HIS:HE1  | 2:N:421:GLY:O    | 1.94                     | 0.50              |
| 1:A:284:ASN:ND2  | 1:A:286:LEU:HG   | 2.26                     | 0.50              |
| 2:O:403:LEU:O    | 2:O:452:MET:HE1  | 2.11                     | 0.50              |
| 2:O:473:LYS:HA   | 2:O:476:GLU:HB2  | 1.94                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 1:C:577[A]:VAL:HG13 | 1:C:649:LEU:HD23 | 1.92                     | 0.50              |
| 2:O:346:ARG:HH22    | 2:O:381:LYS:HZ2  | 1.60                     | 0.50              |
| 2:O:489:ASP:OD1     | 2:O:489:ASP:O    | 2.30                     | 0.50              |
| 1:B:569:VAL:HA      | 1:B:672:GLN:HE22 | 1.77                     | 0.50              |
| 2:M:587:LEU:HD23    | 2:M:588:MET:CE   | 2.42                     | 0.50              |
| 2:N:13:PRO:HB2      | 2:N:16:LYS:HG3   | 1.93                     | 0.50              |
| 2:O:66:ARG:O        | 2:O:70:GLY:HA2   | 2.12                     | 0.50              |
| 2:O:316:ILE:CG1     | 2:O:454:GLU:HG3  | 2.41                     | 0.50              |
| 2:O:417:LEU:HD22    | 2:O:444:TYR:HE1  | 1.76                     | 0.50              |
| 2:P:266:ALA:O       | 2:P:269:ALA:HB3  | 2.11                     | 0.50              |
| 2:M:67:CYS:HB2      | 2:M:227:MET:HE2  | 1.93                     | 0.50              |
| 2:P:516:HIS:HE1     | 2:P:593:THR:O    | 1.94                     | 0.50              |
| 1:C:577[A]:VAL:HG13 | 1:C:649:LEU:CD2  | 2.41                     | 0.50              |
| 1:D:662:VAL:HG21    | 2:P:194:LEU:HD13 | 1.93                     | 0.50              |
| 2:N:243:TYR:CZ      | 2:N:247:ARG:HD3  | 2.46                     | 0.50              |
| 2:O:17:GLU:OE1      | 2:O:22:PHE:HE2   | 1.95                     | 0.50              |
| 2:M:219:ALA:O       | 2:M:223:LEU:HG   | 2.12                     | 0.50              |
| 2:N:568:ASN:ND2     | 2:N:581:GLN:HE21 | 2.09                     | 0.50              |
| 2:O:481:ALA:O       | 2:O:485:TYR:HB2  | 2.12                     | 0.50              |
| 2:N:124:ASP:OD1     | 2:N:125:GLU:OE1  | 2.30                     | 0.49              |
| 2:O:344:GLY:O       | 2:O:345:ASN:OD1  | 2.30                     | 0.49              |
| 2:O:420:THR:OG1     | 2:O:427:TRP:CE3  | 2.30                     | 0.49              |
| 1:C:201:HIS:HE1     | 1:C:627:VAL:HG13 | 1.77                     | 0.49              |
| 1:C:220:HIS:CD2     | 1:C:221:MET:O    | 2.55                     | 0.49              |
| 1:D:260:GLN:NE2     | 10:D:1320:HOH:O  | 2.43                     | 0.49              |
| 2:O:373:ILE:HG12    | 2:O:435:VAL:HG21 | 1.94                     | 0.49              |
| 2:O:470:ASP:O       | 2:O:474:VAL:CG1  | 2.60                     | 0.49              |
| 2:P:4:PHE:CB        | 2:P:238:GLU:OE2  | 2.57                     | 0.49              |
| 1:C:114:CYS:HB2     | 10:C:1242:HOH:O  | 2.11                     | 0.49              |
| 2:N:471:GLU:O       | 2:N:471:GLU:HG3  | 2.10                     | 0.49              |
| 2:P:657:PHE:CE1     | 2:P:667:ILE:HD11 | 2.47                     | 0.49              |
| 1:A:333:SER:CB      | 1:A:503:GLN:HE21 | 2.25                     | 0.49              |
| 2:O:491:ARG:NH1     | 2:O:491:ARG:N    | 2.58                     | 0.49              |
| 1:D:35:GLU:OE2      | 1:D:423:ILE:CD1  | 2.60                     | 0.49              |
| 2:M:540:TYR:CD1     | 2:M:550:PRO:HD3  | 2.47                     | 0.49              |
| 2:O:534:LEU:HD13    | 10:O:1263:HOH:O  | 2.13                     | 0.49              |
| 1:C:69:ARG:HG2      | 1:C:75:PRO:HB3   | 1.94                     | 0.49              |
| 1:D:559:LEU:O       | 1:D:563:MET:HG3  | 2.12                     | 0.49              |
| 2:P:64:VAL:HG13     | 2:P:111:GLU:OE2  | 2.12                     | 0.49              |
| 2:M:169:LEU:HD13    | 2:M:193:LEU:CD2  | 2.42                     | 0.49              |
| 2:M:602:MET:CE      | 2:M:647:ILE:CD1  | 2.74                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:N:160:LEU:HD13   | 2:N:215:ILE:HD13 | 1.94                     | 0.49              |
| 2:P:389:ASP:HB2    | 2:P:464:GLN:HG3  | 1.94                     | 0.49              |
| 1:A:284:ASN:ND2    | 1:A:286:LEU:H    | 2.04                     | 0.49              |
| 1:B:149:ARG:NH2    | 1:B:250:ASP:OD2  | 2.31                     | 0.49              |
| 2:O:476:GLU:OE1    | 2:O:476:GLU:O    | 2.30                     | 0.49              |
| 2:M:427:TRP:C      | 2:M:428:LEU:HD12 | 2.38                     | 0.49              |
| 2:N:486[B]:LYS:HG3 | 2:N:487:GLU:N    | 2.27                     | 0.49              |
| 2:N:489:ASP:O      | 2:N:493:ARG:HG2  | 2.13                     | 0.49              |
| 2:O:59:ALA:HB2     | 2:O:630:THR:HA   | 1.94                     | 0.49              |
| 1:D:201:HIS:HE1    | 2:P:35:TYR:OH    | 1.96                     | 0.49              |
| 2:N:316:ILE:O      | 2:N:316:ILE:HG23 | 2.13                     | 0.49              |
| 1:B:107:LEU:HD21   | 1:B:215:LEU:HB3  | 1.94                     | 0.48              |
| 1:C:614:ASP:N      | 5:C:863:GOL:H32  | 2.24                     | 0.48              |
| 1:B:291:ILE:HD13   | 1:B:397:ALA:HB1  | 1.95                     | 0.48              |
| 1:D:215:LEU:HD22   | 1:D:234:ALA:HA   | 1.95                     | 0.48              |
| 2:N:468:PHE:HB2    | 2:N:474:VAL:HG22 | 1.95                     | 0.48              |
| 2:N:522:PRO:HD3    | 2:N:533:TRP:CD1  | 2.49                     | 0.48              |
| 2:O:344:GLY:H      | 2:O:349:ALA:HB2  | 1.78                     | 0.48              |
| 2:O:503:PHE:CZ     | 2:O:521:THR:HG22 | 2.48                     | 0.48              |
| 2:P:341:GLU:HG3    | 2:P:429:ARG:HG2  | 1.95                     | 0.48              |
| 2:N:63:PRO:HB2     | 2:N:220:ASN:HB2  | 1.95                     | 0.48              |
| 2:O:354:ARG:O      | 2:O:390:ILE:N    | 2.42                     | 0.48              |
| 2:O:468:PHE:CZ     | 2:O:477:TYR:OH   | 2.59                     | 0.48              |
| 2:O:724:THR:C      | 2:O:725:MET:O    | 2.50                     | 0.48              |
| 1:D:658:VAL:O      | 1:D:662:VAL:HG23 | 2.13                     | 0.48              |
| 2:N:424:ASN:H      | 2:N:424:ASN:HD22 | 1.61                     | 0.48              |
| 2:O:393:ARG:NH1    | 2:O:394:LYS:HG2  | 2.29                     | 0.48              |
| 2:O:418:TRP:HH2    | 2:O:420:THR:HG21 | 1.68                     | 0.48              |
| 2:P:150:ASP:OD2    | 2:P:152:THR:HG23 | 2.14                     | 0.48              |
| 2:P:343:GLY:HA2    | 2:P:347:THR:O    | 2.13                     | 0.48              |
| 2:M:320:LEU:HB3    | 2:M:321:PRO:CD   | 2.40                     | 0.48              |
| 2:N:391:TYR:C      | 2:N:391:TYR:CD2  | 2.91                     | 0.48              |
| 2:O:669:TRP:HA     | 2:O:700:ALA:O    | 2.13                     | 0.48              |
| 1:B:201:HIS:CE1    | 2:N:35:TYR:OH    | 2.67                     | 0.48              |
| 1:B:288:SER:O      | 1:B:292:VAL:HG23 | 2.12                     | 0.48              |
| 1:B:606:THR:C      | 1:B:636:MET:HE2  | 2.39                     | 0.48              |
| 1:D:515:ASN:HA     | 1:D:518:THR:CG2  | 2.42                     | 0.48              |
| 1:D:539:ILE:CG2    | 1:D:540:GLY:H    | 2.27                     | 0.48              |
| 2:M:604:ILE:HG13   | 2:M:643:GLY:O    | 2.14                     | 0.48              |
| 2:N:497:ASP:OD2    | 2:N:585:TYR:OH   | 2.24                     | 0.48              |
| 2:O:428:LEU:N      | 2:O:428:LEU:CD2  | 2.76                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:19:VAL:HG22    | 1:A:474:LYS:HG2    | 1.96                     | 0.48              |
| 1:B:368:HIS:CD2    | 1:B:416:ARG:HD2    | 2.48                     | 0.48              |
| 1:D:267:ASN:O      | 1:D:270:VAL:HG22   | 2.13                     | 0.48              |
| 2:P:505:SER:CB     | 2:P:570:TYR:CE2    | 2.95                     | 0.48              |
| 1:C:316:CYS:H      | 1:C:503:GLN:HE22   | 1.62                     | 0.48              |
| 2:O:348:PRO:HG3    | 2:O:475:LYS:CE     | 2.43                     | 0.48              |
| 2:O:487:GLU:O      | 2:O:490:ASP:CG     | 2.57                     | 0.48              |
| 2:P:338:MET:SD     | 2:P:341:GLU:HB2    | 2.54                     | 0.48              |
| 2:M:670:MET:HE3    | 2:M:675:LYS:HG3    | 1.96                     | 0.48              |
| 2:N:609:ASN:ND2    | 2:N:666:ARG:NH1    | 2.61                     | 0.48              |
| 2:O:430:VAL:CG1    | 2:O:434:ALA:HB3    | 2.43                     | 0.48              |
| 2:O:657:PHE:O      | 2:O:658:ILE:C      | 2.57                     | 0.48              |
| 1:C:615:LEU:C      | 1:C:615:LEU:CD2    | 2.85                     | 0.47              |
| 1:D:28:THR:OG1     | 1:D:477:GLN:NE2    | 2.44                     | 0.47              |
| 1:D:282:GLY:HA3    | 1:D:352:ASP:OD1    | 2.14                     | 0.47              |
| 2:M:64:VAL:HA      | 2:M:223:LEU:HD12   | 1.96                     | 0.47              |
| 2:N:4:PHE:N        | 2:N:238[B]:GLU:OE1 | 2.43                     | 0.47              |
| 2:N:312:LYS:NZ     | 2:N:312:LYS:HB3    | 2.29                     | 0.47              |
| 2:O:344:GLY:N      | 2:O:349:ALA:HB2    | 2.29                     | 0.47              |
| 2:O:348:PRO:HG3    | 2:O:475:LYS:HE2    | 1.90                     | 0.47              |
| 2:O:371:PRO:HD2    | 2:O:469:THR:CB     | 2.41                     | 0.47              |
| 2:P:226:GLY:HA3    | 10:P:1355:HOH:O    | 2.13                     | 0.47              |
| 2:O:169:LEU:CD1    | 2:O:193:LEU:HG     | 2.45                     | 0.47              |
| 2:O:490:ASP:O      | 2:O:493:ARG:N      | 2.42                     | 0.47              |
| 2:O:491:ARG:CZ     | 2:O:491:ARG:HB2    | 2.43                     | 0.47              |
| 1:A:217:ASN:ND2    | 1:B:112:ALA:HA     | 2.28                     | 0.47              |
| 1:B:661[A]:GLU:HG3 | 1:B:665:ARG:NH2    | 2.30                     | 0.47              |
| 2:M:615:THR:HG21   | 2:M:674:LEU:HG     | 1.96                     | 0.47              |
| 2:O:376:ILE:CG2    | 2:O:382:LEU:HD21   | 2.37                     | 0.47              |
| 2:O:382:LEU:O      | 2:O:383:PRO:C      | 2.57                     | 0.47              |
| 1:B:486:LYS:HE2    | 1:B:519:TYR:CE2    | 2.49                     | 0.47              |
| 1:D:186:LEU:CD2    | 1:D:205:PRO:HD2    | 2.44                     | 0.47              |
| 2:O:523:GLU:HB3    | 2:O:654:SER:OG     | 2.15                     | 0.47              |
| 2:P:351:GLU:CG     | 2:P:426:ASN:HD21   | 2.27                     | 0.47              |
| 1:C:635:GLU:C      | 1:C:636:MET:HE3    | 2.40                     | 0.47              |
| 2:N:167:LYS:HG2    | 10:N:1288:HOH:O    | 2.14                     | 0.47              |
| 2:O:351:GLU:HB3    | 2:O:423:ARG:H      | 1.70                     | 0.47              |
| 2:O:477:TYR:O      | 2:O:478:MET:C      | 2.58                     | 0.47              |
| 2:O:604:ILE:HA     | 2:O:611:ILE:HG22   | 1.95                     | 0.47              |
| 2:O:653:VAL:O      | 2:O:685:ARG:CD     | 2.56                     | 0.47              |
| 1:D:201:HIS:CE1    | 2:P:35:TYR:OH      | 2.68                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:609:ASN:HD21 | 2:N:666:ARG:HH12 | 1.60                     | 0.47              |
| 2:O:279:ASP:C    | 2:O:279:ASP:OD1  | 2.57                     | 0.47              |
| 2:O:352:LEU:HD11 | 2:O:484:LYS:HG3  | 1.95                     | 0.47              |
| 2:O:480:VAL:O    | 2:O:481:ALA:O    | 2.32                     | 0.47              |
| 1:B:298:MET:HE1  | 1:B:402:ARG:HG2  | 1.95                     | 0.47              |
| 1:C:59:CYS:HB3   | 1:D:75:PRO:HG2   | 1.96                     | 0.47              |
| 2:O:342:MET:HG3  | 2:O:384:LEU:HD23 | 1.97                     | 0.47              |
| 2:O:431:SER:HB3  | 2:O:434:ALA:HB2  | 1.97                     | 0.47              |
| 2:O:594:SER:O    | 2:O:636:GLY:HA2  | 2.14                     | 0.47              |
| 1:A:201:HIS:HE1  | 2:M:35:TYR:OH    | 1.98                     | 0.47              |
| 1:C:331:VAL:HG13 | 1:C:332:THR:N    | 2.30                     | 0.47              |
| 1:D:510:LEU:N    | 1:D:510:LEU:CD1  | 2.77                     | 0.47              |
| 2:O:138:ASP:N    | 2:O:139:PRO:CD   | 2.78                     | 0.47              |
| 2:P:373:ILE:HD12 | 2:P:441:PHE:CE2  | 2.50                     | 0.47              |
| 2:P:402:VAL:HG21 | 2:P:538:ALA:HB2  | 1.94                     | 0.47              |
| 1:A:209:HIS:HD2  | 1:B:213:SER:CB   | 2.28                     | 0.47              |
| 1:A:357:MET:O    | 1:A:360:ILE:HG12 | 2.14                     | 0.47              |
| 2:O:510:GLN:NE2  | 2:O:516:HIS:O    | 2.39                     | 0.47              |
| 2:O:650:THR:O    | 2:O:650:THR:CG2  | 2.60                     | 0.47              |
| 1:C:293:GLN:HG2  | 10:C:1184:HOH:O  | 2.14                     | 0.47              |
| 2:M:540:TYR:O    | 2:M:544:HIS:HD2  | 1.97                     | 0.47              |
| 2:P:124:ASP:OD1  | 2:P:125:GLU:OE1  | 2.33                     | 0.47              |
| 2:P:341:GLU:HG2  | 2:P:428:LEU:O    | 2.14                     | 0.47              |
| 2:P:346:ARG:HH11 | 2:P:346:ARG:HB2  | 1.80                     | 0.47              |
| 2:M:670:MET:SD   | 2:M:674:LEU:HD13 | 2.55                     | 0.46              |
| 2:O:477:TYR:O    | 2:O:480:VAL:N    | 2.41                     | 0.46              |
| 2:O:622:THR:OG1  | 2:O:626:MET:O    | 2.26                     | 0.46              |
| 1:B:182:GLU:HG2  | 1:B:204:VAL:HG11 | 1.97                     | 0.46              |
| 1:C:186:LEU:CD2  | 1:C:205:PRO:HD2  | 2.45                     | 0.46              |
| 1:D:28:THR:HG21  | 1:D:33:VAL:CG1   | 2.44                     | 0.46              |
| 2:N:178:GLY:HA3  | 2:N:317:LYS:HE2  | 1.97                     | 0.46              |
| 1:B:114:CYS:SG   | 1:B:209:HIS:NE2  | 2.89                     | 0.46              |
| 1:C:62:GLY:HA3   | 3:C:700:SF4:S4   | 2.55                     | 0.46              |
| 2:O:95:ASN:ND2   | 2:O:95:ASN:C     | 2.74                     | 0.46              |
| 2:P:275:PRO:CD   | 2:P:309:ARG:HD3  | 2.45                     | 0.46              |
| 1:D:313:VAL:HG21 | 1:D:331:VAL:CG1  | 2.46                     | 0.46              |
| 2:O:150:ASP:OD2  | 2:O:152:THR:HG23 | 2.14                     | 0.46              |
| 2:O:590:ASN:N    | 2:O:591:PRO:HD3  | 2.30                     | 0.46              |
| 2:P:602:MET:HE3  | 2:P:645:MET:HE3  | 1.97                     | 0.46              |
| 2:N:64:VAL:HA    | 2:N:223:LEU:HD12 | 1.96                     | 0.46              |
| 2:O:612:MET:SD   | 2:O:622:THR:HB   | 2.56                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:482:ARG:HA   | 2:P:485:TYR:CD1  | 2.50                     | 0.46              |
| 2:P:700:ALA:HA   | 2:P:704:ILE:HD13 | 1.98                     | 0.46              |
| 1:D:317:CYS:O    | 1:D:321:GLU:HG2  | 2.14                     | 0.46              |
| 1:D:330:LEU:HD23 | 10:D:946:HOH:O   | 2.15                     | 0.46              |
| 1:D:415:ASN:OD1  | 1:D:417:PRO:HD3  | 2.16                     | 0.46              |
| 1:D:594:TRP:CE3  | 1:D:598:LEU:HD12 | 2.51                     | 0.46              |
| 2:O:13:PRO:HB2   | 2:O:16:LYS:HB2   | 1.97                     | 0.46              |
| 2:O:61:TYR:HD1   | 2:O:66:ARG:HD2   | 1.81                     | 0.46              |
| 1:D:432:SER:HA   | 1:D:555:ARG:HD3  | 1.98                     | 0.46              |
| 1:D:617:TYR:O    | 1:D:621:THR:OG1  | 2.32                     | 0.46              |
| 1:D:636:MET:HE2  | 10:D:810:HOH:O   | 2.15                     | 0.46              |
| 2:N:351:GLU:OE2  | 2:N:422:GLN:HA   | 2.16                     | 0.46              |
| 2:N:568:ASN:HD21 | 2:N:581:GLN:HE21 | 1.64                     | 0.46              |
| 2:O:271:PHE:CD2  | 2:O:271:PHE:C    | 2.94                     | 0.46              |
| 1:B:466:LEU:HD22 | 1:B:595:TRP:CZ2  | 2.51                     | 0.46              |
| 2:M:342:MET:HB3  | 2:M:382:LEU:O    | 2.16                     | 0.46              |
| 2:M:457:PRO:O    | 2:M:458:ALA:CB   | 2.64                     | 0.46              |
| 2:M:704:ILE:HG13 | 2:M:705:GLY:N    | 2.30                     | 0.46              |
| 2:O:266:ALA:O    | 2:O:269:ALA:HB3  | 2.15                     | 0.46              |
| 2:O:430:VAL:CG1  | 2:O:431:SER:N    | 2.79                     | 0.46              |
| 1:A:61:ILE:HD13  | 1:A:77:ARG:HD2   | 1.97                     | 0.46              |
| 1:A:584:MET:HG3  | 1:B:73:ALA:HB2   | 1.97                     | 0.46              |
| 1:C:217:ASN:ND2  | 1:D:112:ALA:HA   | 2.31                     | 0.46              |
| 2:M:344:GLY:O    | 2:M:345:ASN:HB2  | 2.16                     | 0.46              |
| 2:O:199:LYS:HD2  | 2:O:204:TYR:OH   | 2.16                     | 0.46              |
| 2:O:343:GLY:HA2  | 2:O:349:ALA:CB   | 2.42                     | 0.46              |
| 2:O:427:TRP:NE1  | 2:O:429:ARG:NH2  | 2.64                     | 0.46              |
| 2:P:138:ASP:N    | 2:P:139:PRO:CD   | 2.79                     | 0.46              |
| 1:B:118:ASN:C    | 1:B:118:ASN:HD22 | 2.23                     | 0.46              |
| 1:B:305:ALA:HB1  | 1:B:409:LYS:HE3  | 1.97                     | 0.46              |
| 1:D:138:LYS:HG3  | 1:D:255:LEU:O    | 2.16                     | 0.46              |
| 2:M:728:ILE:O    | 2:M:729:MET:HB2  | 2.15                     | 0.46              |
| 2:O:337:ASP:O    | 2:O:432:LYS:N    | 2.49                     | 0.46              |
| 2:O:385:GLY:N    | 2:O:474:VAL:CG2  | 2.78                     | 0.46              |
| 2:O:471:GLU:O    | 2:O:475:LYS:HB2  | 2.15                     | 0.46              |
| 2:O:374:ASP:HB3  | 2:O:440:ARG:CZ   | 2.46                     | 0.45              |
| 2:P:313:LEU:HD13 | 2:P:315:LYS:HB2  | 1.99                     | 0.45              |
| 2:P:588:MET:HE3  | 2:P:728:ILE:HG12 | 1.98                     | 0.45              |
| 1:C:383:ALA:O    | 2:P:87:ARG:HD3   | 2.16                     | 0.45              |
| 2:O:318:LEU:HD12 | 2:O:320:LEU:HD21 | 1.97                     | 0.45              |
| 2:O:360:GLU:O    | 2:O:361:ILE:HG22 | 2.15                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:516:HIS:HD2  | 2:O:593:THR:OG1  | 1.98                     | 0.45              |
| 2:O:653:VAL:C    | 2:O:685:ARG:HD2  | 2.39                     | 0.45              |
| 2:P:61:TYR:HD1   | 2:P:66:ARG:HD2   | 1.81                     | 0.45              |
| 2:P:124:ASP:OD2  | 2:P:124:ASP:N    | 2.41                     | 0.45              |
| 2:P:420:THR:HG23 | 2:P:427:TRP:HB3  | 1.98                     | 0.45              |
| 2:P:457:PRO:O    | 2:P:458:ALA:CB   | 2.64                     | 0.45              |
| 1:A:126:GLU:HG2  | 1:A:131:LYS:HB2  | 1.97                     | 0.45              |
| 1:A:299:GLU:O    | 1:A:303:LYS:HG3  | 2.15                     | 0.45              |
| 2:M:333:ILE:HD12 | 2:M:418:TRP:HB2  | 1.98                     | 0.45              |
| 2:M:477:TYR:C    | 2:M:479:GLU:H    | 2.25                     | 0.45              |
| 2:O:474:VAL:HG13 | 2:O:475:LYS:N    | 2.30                     | 0.45              |
| 2:O:670:MET:O    | 2:O:701:ASP:HB3  | 2.16                     | 0.45              |
| 2:P:420:THR:CG2  | 2:P:427:TRP:HB3  | 2.46                     | 0.45              |
| 2:M:587:LEU:HB3  | 2:M:588:MET:HE2  | 1.98                     | 0.45              |
| 2:N:353:VAL:HG22 | 2:N:388:VAL:HB   | 1.98                     | 0.45              |
| 2:O:7:ILE:HD13   | 2:O:245:ARG:HD2  | 1.99                     | 0.45              |
| 1:B:25:ARG:O     | 1:B:49:PHE:HB3   | 2.17                     | 0.45              |
| 1:C:615:LEU:O    | 1:C:619:ILE:HG13 | 2.16                     | 0.45              |
| 1:D:496:VAL:HA   | 1:D:545:PHE:O    | 2.17                     | 0.45              |
| 2:N:433:ASP:OD1  | 2:N:437:LYS:HE2  | 2.16                     | 0.45              |
| 2:O:100:ARG:HB3  | 2:O:271:PHE:HB2  | 1.97                     | 0.45              |
| 2:O:727:PRO:O    | 2:O:729:MET:N    | 2.50                     | 0.45              |
| 1:A:125:VAL:O    | 1:A:129:GLU:HG3  | 2.17                     | 0.45              |
| 1:C:384:TYR:HE2  | 2:P:88:ALA:CB    | 2.29                     | 0.45              |
| 2:O:50:ASP:HA    | 2:O:75:LYS:HD2   | 1.99                     | 0.45              |
| 2:O:232:VAL:HG11 | 2:O:239:GLU:HB3  | 1.97                     | 0.45              |
| 2:O:396:GLN:CD   | 2:O:399:PHE:HD1  | 2.25                     | 0.45              |
| 2:O:585:TYR:CZ   | 2:O:656:LYS:HD2  | 2.52                     | 0.45              |
| 2:O:598:PHE:CE1  | 2:O:601:ILE:HD11 | 2.52                     | 0.45              |
| 2:M:246:ARG:HE   | 2:M:247:ARG:NH1  | 2.14                     | 0.45              |
| 2:O:350:PHE:O    | 2:O:385:GLY:HA2  | 2.16                     | 0.45              |
| 2:O:391:TYR:CE2  | 2:O:462:ARG:HD2  | 2.52                     | 0.45              |
| 1:A:113:HIS:HD1  | 1:A:241:ASP:CG   | 2.23                     | 0.45              |
| 1:A:281:HIS:ND1  | 1:A:282:GLY:N    | 2.65                     | 0.45              |
| 1:A:515:ASN:ND2  | 1:A:518:THR:HG21 | 2.32                     | 0.45              |
| 2:M:657:PHE:O    | 2:M:663:GLY:HA2  | 2.17                     | 0.45              |
| 2:N:66:ARG:O     | 2:N:70:GLY:HA2   | 2.17                     | 0.45              |
| 2:N:384:LEU:CD1  | 2:N:467:ILE:CG2  | 2.93                     | 0.45              |
| 1:C:238:ALA:O    | 1:C:241:ASP:HB3  | 2.17                     | 0.45              |
| 1:C:468:CYS:HB2  | 10:C:693:HOH:O   | 2.17                     | 0.45              |
| 2:M:169:LEU:HD13 | 2:M:193:LEU:HG   | 1.99                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:P:417:LEU:HD21   | 2:P:439:PHE:CE1  | 2.52                     | 0.45              |
| 1:D:515:ASN:OD1    | 1:D:518:THR:HG21 | 2.17                     | 0.44              |
| 2:M:420:THR:HG22   | 2:M:427:TRP:HB3  | 1.97                     | 0.44              |
| 2:N:247:ARG:NH2    | 2:N:514:PRO:HG3  | 2.32                     | 0.44              |
| 2:P:361:ILE:HA     | 2:P:464:GLN:OE1  | 2.16                     | 0.44              |
| 1:B:406:GLU:O      | 1:B:410:GLU:HG3  | 2.17                     | 0.44              |
| 1:C:283:HIS:CD2    | 1:C:317:CYS:CB   | 2.98                     | 0.44              |
| 1:D:261:PRO:HG3    | 1:D:431:TRP:CZ3  | 2.53                     | 0.44              |
| 2:M:604:ILE:HA     | 2:M:611:ILE:HG22 | 1.99                     | 0.44              |
| 2:N:342:MET:HG2    | 2:N:384:LEU:HB2  | 1.98                     | 0.44              |
| 2:O:71:GLU:HG3     | 2:O:82:ILE:CD1   | 2.46                     | 0.44              |
| 2:O:146:ILE:O      | 2:O:146:ILE:HG13 | 2.17                     | 0.44              |
| 2:O:370:GLY:CA     | 2:O:469:THR:OG1  | 2.58                     | 0.44              |
| 1:A:201:HIS:HE1    | 1:A:627:VAL:HG13 | 1.82                     | 0.44              |
| 2:P:357:SER:O      | 2:P:361:ILE:HG22 | 2.17                     | 0.44              |
| 2:P:426:ASN:O      | 2:P:427:TRP:HB2  | 2.16                     | 0.44              |
| 1:B:515:ASN:CA     | 1:B:518:THR:HG23 | 2.47                     | 0.44              |
| 2:M:317:LYS:HE2    | 10:M:862:HOH:O   | 2.18                     | 0.44              |
| 2:M:712:LEU:HB3    | 2:M:713:PRO:HD3  | 1.98                     | 0.44              |
| 2:O:657:PHE:CE1    | 2:O:667:ILE:HD11 | 2.52                     | 0.44              |
| 1:B:238:ALA:O      | 1:B:241:ASP:HB3  | 2.18                     | 0.44              |
| 2:M:651:TYR:O      | 2:M:654:SER:HB3  | 2.18                     | 0.44              |
| 2:O:519:ILE:CG2    | 2:O:584:LEU:HD21 | 2.48                     | 0.44              |
| 1:C:201:HIS:CE1    | 1:C:627:VAL:HG13 | 2.53                     | 0.44              |
| 2:M:187:ASP:HA     | 2:M:211:ASN:HD22 | 1.82                     | 0.44              |
| 2:P:117[B]:ARG:HG2 | 2:P:127:LEU:HD13 | 2.00                     | 0.44              |
| 1:D:284:ASN:HD22   | 1:D:284:ASN:C    | 2.26                     | 0.44              |
| 1:D:455:ALA:HB1    | 1:D:460:GLU:HG3  | 1.98                     | 0.44              |
| 2:P:318:LEU:HD13   | 2:P:320:LEU:CD1  | 2.47                     | 0.44              |
| 1:C:126[A]:GLU:HG2 | 1:C:131:LYS:HB2  | 1.98                     | 0.44              |
| 1:C:149:ARG:HG2    | 1:C:149:ARG:HH11 | 1.83                     | 0.44              |
| 1:C:384:TYR:CE2    | 2:P:88:ALA:HB2   | 2.53                     | 0.44              |
| 2:M:560:ILE:O      | 10:M:1386:HOH:O  | 2.21                     | 0.44              |
| 2:N:490:ASP:HA     | 2:N:493:ARG:HD2  | 2.00                     | 0.44              |
| 2:O:727:PRO:O      | 2:O:728:ILE:C    | 2.61                     | 0.44              |
| 1:B:186:LEU:HD22   | 1:B:205:PRO:HD2  | 2.00                     | 0.44              |
| 1:B:601:PRO:HD3    | 1:B:652:ARG:CZ   | 2.48                     | 0.44              |
| 2:M:236:ALA:O      | 2:M:240:GLN:HG2  | 2.18                     | 0.44              |
| 2:O:396:GLN:OE1    | 2:O:398:ASP:N    | 2.49                     | 0.44              |
| 2:P:385:GLY:O      | 2:P:467:ILE:HA   | 2.17                     | 0.44              |
| 2:P:589:GLU:O      | 2:P:590:ASN:C    | 2.60                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:39:LYS:O      | 1:A:42:ASP:HB2     | 2.17                     | 0.43              |
| 2:M:602:MET:HE2   | 2:M:602:MET:HB3    | 1.95                     | 0.43              |
| 2:N:45:ARG:HD2    | 10:N:1293:HOH:O    | 2.18                     | 0.43              |
| 2:O:584:LEU:HD23  | 2:O:592:MET:HE1    | 1.99                     | 0.43              |
| 1:C:213:SER:CB    | 1:D:209:HIS:CD2    | 2.97                     | 0.43              |
| 1:D:331:VAL:HG23  | 1:D:332:THR:H      | 1.82                     | 0.43              |
| 1:D:358:PRO:HA    | 1:D:380:ILE:HD13   | 2.00                     | 0.43              |
| 1:D:450:ARG:O     | 1:D:450:ARG:HG3    | 2.18                     | 0.43              |
| 2:N:11:ALA:O      | 2:N:13:PRO:HD3     | 2.18                     | 0.43              |
| 2:N:26:TYR:CE2    | 2:N:30:ILE:HD11    | 2.52                     | 0.43              |
| 2:N:355:THR:HG23  | 2:N:395:MET:HG2    | 2.00                     | 0.43              |
| 2:O:169:LEU:HD13  | 2:O:193:LEU:HG     | 2.01                     | 0.43              |
| 2:O:473:LYS:O     | 2:O:476:GLU:N      | 2.45                     | 0.43              |
| 1:A:657:GLY:O     | 1:A:661[A]:GLU:HG3 | 2.18                     | 0.43              |
| 2:N:184:PHE:C     | 2:N:185:ILE:HG13   | 2.42                     | 0.43              |
| 2:O:232:VAL:HG13  | 2:O:239:GLU:HB3    | 1.99                     | 0.43              |
| 2:O:315:LYS:O     | 2:O:316:ILE:HB     | 2.18                     | 0.43              |
| 2:O:462:ARG:O     | 2:O:463:VAL:HG23   | 2.19                     | 0.43              |
| 2:P:358:GLU:O     | 2:P:462:ARG:NH2    | 2.51                     | 0.43              |
| 2:P:576:ASN:O     | 2:P:577:ARG:HB2    | 2.18                     | 0.43              |
| 2:P:678:LEU:O     | 2:P:679:HIS:C      | 2.61                     | 0.43              |
| 2:P:711:ILE:O     | 2:P:714:TYR:HB3    | 2.18                     | 0.43              |
| 1:A:492:ASN:HA    | 1:A:524:LEU:HB2    | 2.00                     | 0.43              |
| 1:C:278:PHE:HB3   | 1:C:312:LEU:HD23   | 1.99                     | 0.43              |
| 1:D:107:LEU:HD21  | 1:D:215:LEU:HB3    | 2.00                     | 0.43              |
| 1:D:351:VAL:HB    | 1:D:356:ILE:HD13   | 2.01                     | 0.43              |
| 2:M:3:ASP:O       | 2:M:6[A]:LYS:HB3   | 2.18                     | 0.43              |
| 2:O:444:TYR:O     | 2:O:448:LEU:HD22   | 2.18                     | 0.43              |
| 2:N:193:LEU:O     | 2:N:198:VAL:HG13   | 2.18                     | 0.43              |
| 2:N:324:PHE:HA    | 2:N:413:TYR:O      | 2.19                     | 0.43              |
| 1:A:297:GLU:OE1   | 1:A:398:LYS:NZ     | 2.42                     | 0.43              |
| 1:D:453:ASN:ND2   | 1:D:566:ASP:HB3    | 2.34                     | 0.43              |
| 2:M:583:CYS:HB3   | 2:M:586:THR:HG22   | 2.00                     | 0.43              |
| 2:N:604:ILE:HB    | 2:N:606:PRO:HD3    | 2.01                     | 0.43              |
| 2:P:504:TYR:CE2   | 2:P:550:PRO:HB3    | 2.54                     | 0.43              |
| 1:A:186:LEU:HD22  | 1:A:205:PRO:HD2    | 2.01                     | 0.43              |
| 1:B:414:SER:O     | 1:B:415:ASN:HB2    | 2.18                     | 0.43              |
| 1:B:661[A]:GLU:CG | 1:B:665:ARG:HH21   | 2.32                     | 0.43              |
| 1:C:401:ILE:O     | 1:C:405:ILE:HG13   | 2.18                     | 0.43              |
| 2:M:244:GLN:HG3   | 2:M:272:THR:CG2    | 2.48                     | 0.43              |
| 2:N:560:ILE:N     | 2:N:560:ILE:HD13   | 2.32                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:51:HIS:HA    | 2:O:52:PRO:HD3   | 1.86                     | 0.43              |
| 2:O:373:ILE:HG22 | 2:O:440:ARG:HG3  | 1.99                     | 0.43              |
| 2:O:490:ASP:C    | 2:O:492:MET:N    | 2.76                     | 0.43              |
| 2:O:584:LEU:O    | 2:O:585:TYR:HD2  | 2.01                     | 0.43              |
| 2:P:361:ILE:HG21 | 2:P:391:TYR:HB2  | 2.00                     | 0.43              |
| 1:B:65:GLY:O     | 1:B:97:ILE:HG22  | 2.19                     | 0.43              |
| 1:C:557:VAL:CG2  | 1:C:594:TRP:CZ3  | 3.02                     | 0.43              |
| 2:N:309:ARG:HA   | 2:N:309:ARG:HD2  | 1.87                     | 0.43              |
| 2:N:604:ILE:H    | 2:N:604:ILE:HG13 | 1.57                     | 0.43              |
| 2:O:423:ARG:HG2  | 2:O:423:ARG:HH11 | 1.84                     | 0.43              |
| 2:O:720:HIS:HA   | 2:O:721:PRO:HD3  | 1.95                     | 0.43              |
| 2:M:335:LYS:HG3  | 2:M:429:ARG:HH12 | 1.84                     | 0.43              |
| 2:N:441:PHE:CE1  | 2:N:469:THR:HG21 | 2.54                     | 0.43              |
| 2:O:396:GLN:HG3  | 2:O:399:PHE:CE1  | 2.54                     | 0.43              |
| 2:P:3:ASP:O      | 2:P:6:LYS:HB3    | 2.19                     | 0.43              |
| 1:A:537:ILE:HG22 | 1:A:540:GLY:H    | 1.84                     | 0.43              |
| 1:B:220:HIS:CD2  | 1:B:221:MET:O    | 2.71                     | 0.43              |
| 1:B:308:LYS:HE3  | 1:B:308:LYS:HA   | 2.00                     | 0.43              |
| 1:C:164:GLN:O    | 1:C:168:GLU:HG3  | 2.18                     | 0.43              |
| 1:D:28:THR:HG21  | 1:D:33:VAL:HG12  | 2.00                     | 0.43              |
| 1:D:126:GLU:OE1  | 1:D:390:THR:OG1  | 2.33                     | 0.43              |
| 1:D:416:ARG:O    | 1:D:417:PRO:C    | 2.60                     | 0.43              |
| 2:O:169:LEU:HD13 | 2:O:193:LEU:CG   | 2.49                     | 0.43              |
| 2:P:79:LEU:HD22  | 2:P:112:ILE:HG12 | 2.01                     | 0.43              |
| 1:A:12:ARG:NH2   | 10:A:1449:HOH:O  | 2.52                     | 0.42              |
| 1:A:626:ASP:HB3  | 2:M:212:PHE:CG   | 2.54                     | 0.42              |
| 1:C:622:GLN:O    | 1:C:625:SER:OG   | 2.30                     | 0.42              |
| 1:D:20:MET:O     | 1:D:21:GLU:C     | 2.62                     | 0.42              |
| 2:O:390:ILE:HG22 | 2:O:391:TYR:H    | 1.84                     | 0.42              |
| 2:O:488:ARG:C    | 2:O:490:ASP:N    | 2.77                     | 0.42              |
| 2:P:602:MET:HE1  | 2:P:645:MET:HE3  | 2.01                     | 0.42              |
| 1:C:122:HIS:HD2  | 10:C:869:HOH:O   | 2.01                     | 0.42              |
| 1:C:431:TRP:O    | 1:C:547:MET:HG2  | 2.19                     | 0.42              |
| 1:D:142:LYS:O    | 1:D:143:LEU:C    | 2.59                     | 0.42              |
| 1:D:339:LEU:O    | 1:D:340:ALA:C    | 2.62                     | 0.42              |
| 2:N:657:PHE:O    | 2:N:663:GLY:HA2  | 2.17                     | 0.42              |
| 2:O:587:LEU:HD13 | 2:O:602:MET:HE3  | 2.01                     | 0.42              |
| 2:P:356:VAL:HG21 | 2:P:389:ASP:HB3  | 2.00                     | 0.42              |
| 1:A:220:HIS:CD2  | 1:A:221:MET:O    | 2.70                     | 0.42              |
| 1:C:216:VAL:HG12 | 1:D:108:THR:HA   | 2.00                     | 0.42              |
| 2:M:588:MET:HE3  | 2:M:728:ILE:HG12 | 2.01                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 2:O:478:MET:O       | 2:O:481:ALA:CA   | 2.67                     | 0.42              |
| 2:P:657:PHE:O       | 2:P:663:GLY:HA2  | 2.19                     | 0.42              |
| 1:A:432:SER:HA      | 1:A:555:ARG:HD3  | 2.01                     | 0.42              |
| 1:B:88:GLY:HA3      | 3:B:750:SF4:S3   | 2.60                     | 0.42              |
| 1:B:515:ASN:HA      | 1:B:518:THR:CG2  | 2.47                     | 0.42              |
| 1:A:30:ASP:OD2      | 1:A:507:LYS:NZ   | 2.45                     | 0.42              |
| 1:C:196:GLU:OE2     | 2:O:120:LYS:HE3  | 2.20                     | 0.42              |
| 1:D:18:ARG:CD       | 1:D:636:MET:HE3  | 2.49                     | 0.42              |
| 2:N:354:ARG:HH21    | 2:N:480:VAL:HG11 | 1.83                     | 0.42              |
| 2:O:459:ILE:HD11    | 2:O:542:ILE:HG21 | 1.99                     | 0.42              |
| 2:O:482:ARG:HB3     | 2:O:483:GLU:H    | 1.67                     | 0.42              |
| 2:O:488:ARG:CG      | 2:O:488:ARG:HH11 | 2.32                     | 0.42              |
| 2:O:527:LEU:CD2     | 2:O:594:SER:HA   | 2.49                     | 0.42              |
| 2:P:372:ASP:OD1     | 2:P:373:ILE:N    | 2.42                     | 0.42              |
| 1:A:112:ALA:HA      | 1:B:217:ASN:HD22 | 1.84                     | 0.42              |
| 1:A:622:GLN:O       | 1:A:625:SER:OG   | 2.32                     | 0.42              |
| 1:D:201:HIS:CE1     | 1:D:627:VAL:HG13 | 2.55                     | 0.42              |
| 2:M:247:ARG:NH1     | 10:M:971:HOH:O   | 2.52                     | 0.42              |
| 2:O:493:ARG:HH11    | 2:O:493:ARG:HA   | 1.84                     | 0.42              |
| 1:A:353:VAL:O       | 1:A:354:GLN:HB2  | 2.19                     | 0.42              |
| 1:B:571:THR:N       | 1:B:572:PRO:CD   | 2.83                     | 0.42              |
| 1:C:149:ARG:HG2     | 1:C:149:ARG:NH1  | 2.34                     | 0.42              |
| 1:C:190:ILE:HG13    | 1:C:195:LYS:HG3  | 2.01                     | 0.42              |
| 1:D:573:LYS:HB3     | 1:D:573:LYS:HE3  | 1.89                     | 0.42              |
| 2:M:138:ASP:N       | 2:M:139:PRO:CD   | 2.83                     | 0.42              |
| 2:M:702:GLU:H       | 2:M:702:GLU:HG3  | 1.30                     | 0.42              |
| 2:N:583:CYS:CB      | 2:N:586:THR:HG22 | 2.50                     | 0.42              |
| 2:P:315:LYS:HE3     | 10:P:1084:HOH:O  | 2.19                     | 0.42              |
| 1:B:149:ARG:HD2     | 10:B:1427:HOH:O  | 2.19                     | 0.42              |
| 1:B:298:MET:HE1     | 1:B:402:ARG:CG   | 2.50                     | 0.42              |
| 1:C:213:SER:HB3     | 1:D:209:HIS:CD2  | 2.55                     | 0.42              |
| 1:C:577[A]:VAL:HG21 | 1:C:645:ILE:CG2  | 2.41                     | 0.42              |
| 2:M:339:TYR:HB2     | 2:M:432:LYS:HA   | 2.02                     | 0.42              |
| 2:M:568:ASN:ND2     | 2:M:581:GLN:HE21 | 2.14                     | 0.42              |
| 2:N:339:TYR:CG      | 2:N:435:VAL:HG21 | 2.55                     | 0.42              |
| 2:N:377:PRO:HG2     | 2:N:380:SER:HB3  | 2.00                     | 0.42              |
| 2:O:345:ASN:OD1     | 2:O:345:ASN:C    | 2.61                     | 0.42              |
| 2:O:631:LEU:O       | 2:O:635:ILE:HG23 | 2.19                     | 0.42              |
| 2:P:117[B]:ARG:NH1  | 10:P:1004:HOH:O  | 2.44                     | 0.42              |
| 2:P:431:SER:O       | 2:P:435:VAL:HG23 | 2.19                     | 0.42              |
| 2:P:604:ILE:HD12    | 2:P:610:GLY:O    | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:368:HIS:CE1  | 1:C:416:ARG:CB   | 3.00                     | 0.42              |
| 1:C:482:LEU:HD22 | 1:C:482:LEU:HA   | 1.81                     | 0.42              |
| 1:D:12:ARG:HB3   | 1:D:13:PRO:HD2   | 2.02                     | 0.42              |
| 2:M:7:ILE:CD1    | 2:M:245:ARG:HD2  | 2.43                     | 0.42              |
| 2:M:587:LEU:HD23 | 2:M:588:MET:HE1  | 2.01                     | 0.42              |
| 2:N:71:GLU:HG2   | 2:N:82:ILE:HD11  | 2.02                     | 0.42              |
| 2:N:361:ILE:HD13 | 2:N:391:TYR:HB3  | 2.01                     | 0.42              |
| 2:N:374:ASP:O    | 2:N:375:GLN:HG3  | 2.20                     | 0.42              |
| 2:N:468:PHE:HB2  | 2:N:474:VAL:CG2  | 2.50                     | 0.42              |
| 2:N:674:LEU:HD22 | 2:N:678:LEU:HG   | 2.01                     | 0.42              |
| 1:B:78:ILE:HD11  | 1:B:97:ILE:HD12  | 2.01                     | 0.42              |
| 1:B:218:GLN:HE22 | 1:B:233:SER:CB   | 2.32                     | 0.42              |
| 1:C:274:ASP:HB3  | 1:C:308:LYS:HD3  | 2.02                     | 0.42              |
| 1:D:271:LEU:HD21 | 1:D:331:VAL:HG11 | 2.02                     | 0.42              |
| 1:D:626:ASP:HB3  | 2:P:212:PHE:CG   | 2.55                     | 0.42              |
| 2:O:298:TYR:HA   | 2:O:301:ILE:HG13 | 2.01                     | 0.42              |
| 2:O:581:GLN:O    | 2:O:590:ASN:HB3  | 2.20                     | 0.42              |
| 2:O:627:THR:O    | 2:O:628:PHE:C    | 2.63                     | 0.42              |
| 2:P:542:ILE:HG13 | 2:P:543:ASN:N    | 2.35                     | 0.42              |
| 2:P:579:LEU:HD23 | 2:P:579:LEU:HA   | 1.90                     | 0.42              |
| 2:P:728:ILE:HG23 | 2:P:728:ILE:O    | 2.20                     | 0.42              |
| 2:M:333:ILE:HD12 | 2:M:418:TRP:CB   | 2.50                     | 0.41              |
| 2:M:424:ASN:H    | 2:M:424:ASN:ND2  | 2.14                     | 0.41              |
| 2:O:488:ARG:O    | 2:O:490:ASP:N    | 2.52                     | 0.41              |
| 2:O:584:LEU:O    | 2:O:585:TYR:CD2  | 2.72                     | 0.41              |
| 2:P:17:GLU:HA    | 2:P:18:PRO:HD3   | 1.93                     | 0.41              |
| 2:P:422:GLN:HG2  | 2:P:423:ARG:HG3  | 2.02                     | 0.41              |
| 2:P:594:SER:HB3  | 2:P:598:PHE:HD2  | 1.85                     | 0.41              |
| 2:P:601:ILE:HG21 | 2:P:631:LEU:HG   | 2.01                     | 0.41              |
| 1:C:414:SER:C    | 1:C:416:ARG:N    | 2.75                     | 0.41              |
| 1:D:33:VAL:HG13  | 1:D:339:LEU:CD1  | 2.49                     | 0.41              |
| 1:D:510:LEU:H    | 1:D:510:LEU:CD1  | 2.31                     | 0.41              |
| 2:M:419:HIS:ND1  | 2:M:419:HIS:C    | 2.78                     | 0.41              |
| 2:N:146:ILE:HD11 | 3:N:900:SF4:S1   | 2.60                     | 0.41              |
| 2:N:459:ILE:HD12 | 2:N:542:ILE:HG13 | 2.02                     | 0.41              |
| 2:O:363:ASP:HB2  | 2:O:462:ARG:HG2  | 2.03                     | 0.41              |
| 2:O:422:GLN:N    | 2:O:422:GLN:CD   | 2.78                     | 0.41              |
| 2:O:422:GLN:O    | 2:O:423:ARG:C    | 2.62                     | 0.41              |
| 2:O:474:VAL:CG1  | 2:O:475:LYS:N    | 2.83                     | 0.41              |
| 2:P:500:VAL:O    | 2:P:553:LYS:NZ   | 2.47                     | 0.41              |
| 2:P:541:GLU:H    | 2:P:541:GLU:HG2  | 1.56                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 1:A:200:THR:OG1     | 1:A:201:HIS:HD2  | 2.03                     | 0.41              |
| 1:A:217:ASN:O       | 1:A:223:MET:HG3  | 2.21                     | 0.41              |
| 1:C:221:MET:SD      | 1:C:221:MET:C    | 3.03                     | 0.41              |
| 1:D:615:LEU:H       | 5:D:863:GOL:H12  | 1.84                     | 0.41              |
| 2:M:277:ILE:HG23    | 2:M:295:VAL:HG23 | 2.02                     | 0.41              |
| 2:O:167:LYS:HG2     | 10:O:997:HOH:O   | 2.20                     | 0.41              |
| 2:O:315:LYS:HB2     | 2:O:316:ILE:H    | 1.50                     | 0.41              |
| 2:O:430:VAL:CG1     | 2:O:431:SER:H    | 2.32                     | 0.41              |
| 2:O:552:PRO:O       | 2:O:554:GLU:N    | 2.49                     | 0.41              |
| 2:O:671:PRO:HA      | 2:O:702:GLU:OE1  | 2.20                     | 0.41              |
| 2:P:392:GLY:HA3     | 2:P:459:ILE:O    | 2.20                     | 0.41              |
| 2:P:505:SER:CB      | 2:P:570:TYR:HE2  | 2.31                     | 0.41              |
| 2:P:704:ILE:HG22    | 2:P:711:ILE:HG22 | 2.02                     | 0.41              |
| 1:B:186:LEU:CD2     | 1:B:205:PRO:HD2  | 2.50                     | 0.41              |
| 1:D:69:ARG:HD3      | 1:D:75:PRO:HG3   | 2.02                     | 0.41              |
| 2:M:21:LEU:HB2      | 2:M:286:LYS:HA   | 2.03                     | 0.41              |
| 2:N:16:LYS:HZ3      | 2:N:16:LYS:HB3   | 1.85                     | 0.41              |
| 2:N:156:GLU:HG3     | 2:N:182:MET:HB3  | 2.02                     | 0.41              |
| 2:N:696:ILE:HA      | 2:N:699:ILE:HD12 | 2.02                     | 0.41              |
| 2:O:95:ASN:HD21     | 2:O:98:ASN:H     | 1.67                     | 0.41              |
| 2:O:249:ARG:HA      | 2:O:309:ARG:NH2  | 2.36                     | 0.41              |
| 2:O:388:VAL:HG22    | 2:O:465:VAL:HG13 | 2.01                     | 0.41              |
| 2:O:427:TRP:CE2     | 2:O:429:ARG:NH2  | 2.88                     | 0.41              |
| 2:O:527:LEU:HD22    | 2:O:594:SER:HA   | 2.00                     | 0.41              |
| 2:P:221:TYR:O       | 2:P:222:ALA:C    | 2.61                     | 0.41              |
| 1:C:577[A]:VAL:HG12 | 1:C:601:PRO:HG2  | 2.01                     | 0.41              |
| 1:D:510:LEU:O       | 1:D:543:PRO:HD2  | 2.21                     | 0.41              |
| 2:O:348:PRO:CG      | 2:O:475:LYS:HE3  | 2.46                     | 0.41              |
| 2:O:728:ILE:O       | 2:O:729:MET:O    | 2.38                     | 0.41              |
| 1:B:160:LEU:HD23    | 1:B:160:LEU:HA   | 1.87                     | 0.41              |
| 1:C:61:ILE:HG22     | 1:C:67:CYS:HB2   | 2.02                     | 0.41              |
| 1:C:169:LYS:O       | 1:C:172:GLU:HB2  | 2.21                     | 0.41              |
| 1:D:51:ARG:O        | 1:D:52:PHE:C     | 2.62                     | 0.41              |
| 2:O:343:GLY:C       | 2:O:349:ALA:HB2  | 2.44                     | 0.41              |
| 2:O:360:GLU:O       | 2:O:361:ILE:CG2  | 2.68                     | 0.41              |
| 2:O:396:GLN:CD      | 2:O:399:PHE:CD1  | 2.99                     | 0.41              |
| 2:O:712:LEU:O       | 2:O:715:LEU:N    | 2.54                     | 0.41              |
| 2:P:478:MET:O       | 2:P:482:ARG:HB2  | 2.20                     | 0.41              |
| 1:A:284:ASN:HD22    | 1:A:284:ASN:C    | 2.29                     | 0.41              |
| 1:B:368:HIS:NE2     | 1:B:416:ARG:CD   | 2.84                     | 0.41              |
| 1:B:398:LYS:O       | 1:B:402:ARG:HG3  | 2.21                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:C:235:ILE:HG23   | 1:C:597:SER:OG   | 2.21                     | 0.41              |
| 2:N:350:PHE:HA     | 2:N:423:ARG:O    | 2.20                     | 0.41              |
| 2:O:243:TYR:CD1    | 2:O:243:TYR:C    | 2.98                     | 0.41              |
| 2:O:482:ARG:O      | 2:O:485:TYR:HB3  | 2.20                     | 0.41              |
| 2:P:254:TYR:O      | 2:P:278:THR:HA   | 2.21                     | 0.41              |
| 2:P:581:GLN:O      | 2:P:590:ASN:HB3  | 2.20                     | 0.41              |
| 1:B:467:ILE:O      | 1:B:497:ALA:HA   | 2.20                     | 0.41              |
| 1:C:507:LYS:HB2    | 1:C:507:LYS:HE3  | 1.87                     | 0.41              |
| 1:D:186:LEU:HD22   | 1:D:205:PRO:HD2  | 2.03                     | 0.41              |
| 2:M:315:LYS:O      | 2:M:316:ILE:O    | 2.38                     | 0.41              |
| 2:M:683:VAL:HG13   | 2:M:693:GLU:HA   | 2.03                     | 0.41              |
| 2:O:343:GLY:C      | 2:O:347:THR:O    | 2.64                     | 0.41              |
| 2:O:482:ARG:O      | 2:O:485:TYR:CB   | 2.69                     | 0.41              |
| 1:D:149[B]:ARG:HD2 | 1:D:188:THR:O    | 2.20                     | 0.41              |
| 2:M:169:LEU:HD13   | 2:M:193:LEU:HD21 | 2.03                     | 0.41              |
| 2:O:344:GLY:N      | 2:O:426:ASN:O    | 2.54                     | 0.41              |
| 2:O:488:ARG:NH1    | 2:O:488:ARG:CG   | 2.83                     | 0.41              |
| 2:O:489:ASP:OD1    | 2:O:489:ASP:C    | 2.63                     | 0.41              |
| 2:O:604:ILE:CD1    | 2:O:606:PRO:HD3  | 2.30                     | 0.41              |
| 2:O:661:ASP:O      | 2:O:666:ARG:NE   | 2.32                     | 0.41              |
| 2:P:656:LYS:HA     | 2:P:656:LYS:HD3  | 1.81                     | 0.41              |
| 1:A:78:ILE:HD11    | 1:A:97:ILE:HD12  | 2.03                     | 0.41              |
| 1:A:587:LYS:H      | 1:B:220:HIS:HE1  | 1.68                     | 0.41              |
| 1:B:601:PRO:HB3    | 1:B:631:TYR:CZ   | 2.56                     | 0.41              |
| 1:C:313:VAL:HG12   | 1:C:329:PRO:HG2  | 2.02                     | 0.41              |
| 2:O:187:ASP:HA     | 2:O:211:ASN:HD22 | 1.85                     | 0.41              |
| 2:O:726:ASP:HB2    | 2:O:727:PRO:HD2  | 2.03                     | 0.41              |
| 2:P:187:ASP:HA     | 2:P:211:ASN:HD22 | 1.85                     | 0.41              |
| 1:A:279:VAL:HG22   | 1:A:313:VAL:CG2  | 2.51                     | 0.40              |
| 1:A:469:GLY:C      | 4:A:800:XCC:S1   | 3.04                     | 0.40              |
| 1:C:112:ALA:HA     | 1:D:217:ASN:ND2  | 2.33                     | 0.40              |
| 1:C:197:LYS:HE2    | 1:C:197:LYS:HB2  | 1.88                     | 0.40              |
| 1:D:220:HIS:CD2    | 1:D:221:MET:O    | 2.72                     | 0.40              |
| 5:D:863:GOL:C2     | 2:P:27:HIS:CE1   | 3.00                     | 0.40              |
| 2:M:711:ILE:O      | 2:M:715:LEU:HG   | 2.20                     | 0.40              |
| 2:N:651:TYR:HA     | 10:N:876:HOH:O   | 2.21                     | 0.40              |
| 2:O:61:TYR:CD1     | 2:O:66:ARG:HD2   | 2.55                     | 0.40              |
| 2:O:182:MET:HG3    | 2:O:205:ILE:HG22 | 2.01                     | 0.40              |
| 2:O:281:PRO:HG3    | 2:O:296:GLU:OE2  | 2.21                     | 0.40              |
| 2:O:351:GLU:CG     | 2:O:423:ARG:N    | 2.65                     | 0.40              |
| 2:O:430:VAL:HG12   | 2:O:434:ALA:HB3  | 2.03                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:21:LEU:HB2   | 2:P:286:LYS:HA   | 2.01                     | 0.40              |
| 2:P:494:GLY:N    | 10:P:1094:HOH:O  | 2.34                     | 0.40              |
| 1:A:77:ARG:HB3   | 10:A:1466:HOH:O  | 2.22                     | 0.40              |
| 1:A:235:ILE:HG23 | 1:A:597:SER:OG   | 2.21                     | 0.40              |
| 2:O:351:GLU:O    | 2:O:352:LEU:CB   | 2.65                     | 0.40              |
| 2:O:366:ILE:H    | 2:O:366:ILE:HG13 | 1.74                     | 0.40              |
| 2:O:424:ASN:ND2  | 2:O:485:TYR:HE1  | 2.16                     | 0.40              |
| 2:P:341:GLU:OE1  | 2:P:427:TRP:NE1  | 2.53                     | 0.40              |
| 1:B:652:ARG:O    | 1:B:656:LEU:HB2  | 2.22                     | 0.40              |
| 1:D:170:ALA:O    | 1:D:173:ASP:HB2  | 2.21                     | 0.40              |
| 1:D:201:HIS:HE1  | 1:D:627:VAL:HG13 | 1.86                     | 0.40              |
| 1:D:320:ASN:O    | 1:D:321:GLU:C    | 2.63                     | 0.40              |
| 2:M:199:LYS:HE2  | 2:M:415:GLU:OE2  | 2.22                     | 0.40              |
| 2:M:563:ILE:HD11 | 2:M:583:CYS:SG   | 2.61                     | 0.40              |
| 2:O:111:GLU:HA   | 2:O:216:VAL:HG11 | 2.03                     | 0.40              |
| 2:P:287:GLN:HE22 | 2:P:289:PRO:HG3  | 1.87                     | 0.40              |
| 2:P:427:TRP:C    | 2:P:428:LEU:HD12 | 2.46                     | 0.40              |
| 1:B:662:VAL:HG21 | 2:N:194:LEU:HD13 | 2.03                     | 0.40              |
| 1:C:174:PHE:CE2  | 1:C:208:ILE:HD12 | 2.56                     | 0.40              |
| 1:D:116:HIS:CD2  | 1:D:116:HIS:C    | 3.00                     | 0.40              |
| 1:D:200:THR:OG1  | 1:D:201:HIS:HD2  | 2.05                     | 0.40              |
| 2:M:349:ALA:CB   | 2:M:426:ASN:HD21 | 2.35                     | 0.40              |
| 2:N:604:ILE:HG13 | 2:N:643:GLY:O    | 2.21                     | 0.40              |
| 2:O:484:LYS:HD3  | 2:O:484:LYS:HA   | 1.59                     | 0.40              |
| 1:A:20:MET:HG3   | 10:A:883:HOH:O   | 2.21                     | 0.40              |
| 1:A:440:LEU:HB3  | 1:A:448:PRO:O    | 2.21                     | 0.40              |
| 1:C:384:TYR:HE2  | 2:P:88:ALA:HB2   | 1.86                     | 0.40              |
| 2:M:349:ALA:HB3  | 2:M:426:ASN:HD21 | 1.86                     | 0.40              |
| 2:O:720:HIS:O    | 2:O:723:LEU:N    | 2.54                     | 0.40              |
| 2:P:351:GLU:CD   | 2:P:426:ASN:HD21 | 2.30                     | 0.40              |
| 2:P:442:LYS:HE2  | 2:P:442:LYS:HB2  | 1.66                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|----------|-------------|----|
| 1   | A     | 678/674 (101%)   | 652 (96%)  | 24 (4%)  | 2 (0%)   | 36          | 34 |
| 1   | B     | 676/674 (100%)   | 652 (96%)  | 23 (3%)  | 1 (0%)   | 48          | 50 |
| 1   | C     | 673/674 (100%)   | 648 (96%)  | 24 (4%)  | 1 (0%)   | 48          | 50 |
| 1   | D     | 675/674 (100%)   | 640 (95%)  | 30 (4%)  | 5 (1%)   | 18          | 13 |
| 2   | M     | 731/729 (100%)   | 687 (94%)  | 36 (5%)  | 8 (1%)   | 11          | 7  |
| 2   | N     | 732/729 (100%)   | 689 (94%)  | 34 (5%)  | 9 (1%)   | 10          | 5  |
| 2   | O     | 727/729 (100%)   | 641 (88%)  | 60 (8%)  | 26 (4%)  | 2           | 0  |
| 2   | P     | 727/729 (100%)   | 679 (93%)  | 41 (6%)  | 7 (1%)   | 12          | 8  |
| All | All   | 5619/5612 (100%) | 5288 (94%) | 272 (5%) | 59 (1%)  | 11          | 7  |

All (59) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 267 | ASN  |
| 1   | D     | 267 | ASN  |
| 2   | M     | 316 | ILE  |
| 2   | M     | 693 | GLU  |
| 2   | O     | 315 | LYS  |
| 2   | O     | 316 | ILE  |
| 2   | O     | 317 | LYS  |
| 2   | O     | 361 | ILE  |
| 2   | O     | 397 | ALA  |
| 2   | O     | 482 | ARG  |
| 2   | O     | 485 | TYR  |
| 2   | O     | 486 | LYS  |
| 2   | O     | 492 | MET  |
| 2   | O     | 728 | ILE  |
| 2   | P     | 316 | ILE  |
| 2   | P     | 360 | GLU  |
| 1   | A     | 267 | ASN  |
| 2   | M     | 187 | ASP  |
| 2   | M     | 315 | LYS  |
| 2   | N     | 187 | ASP  |
| 2   | N     | 449 | VAL  |
| 2   | N     | 693 | GLU  |
| 2   | O     | 187 | ASP  |
| 2   | O     | 335 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 470 | ASP  |
| 2   | O     | 555 | GLY  |
| 2   | P     | 458 | ALA  |
| 2   | P     | 679 | HIS  |
| 1   | C     | 267 | ASN  |
| 2   | M     | 596 | GLY  |
| 2   | M     | 658 | ILE  |
| 2   | O     | 436 | ALA  |
| 2   | O     | 489 | ASP  |
| 2   | O     | 650 | THR  |
| 2   | O     | 679 | HIS  |
| 2   | P     | 187 | ASP  |
| 2   | N     | 426 | ASN  |
| 2   | O     | 399 | PHE  |
| 2   | P     | 228 | MET  |
| 2   | P     | 596 | GLY  |
| 1   | A     | 354 | GLN  |
| 1   | D     | 552 | ASP  |
| 2   | N     | 290 | ASP  |
| 2   | O     | 459 | ILE  |
| 2   | O     | 727 | PRO  |
| 1   | D     | 354 | GLN  |
| 1   | D     | 416 | ARG  |
| 1   | D     | 492 | ASN  |
| 2   | M     | 478 | MET  |
| 2   | M     | 719 | GLY  |
| 2   | N     | 596 | GLY  |
| 2   | O     | 484 | LYS  |
| 2   | N     | 316 | ILE  |
| 2   | O     | 382 | LEU  |
| 2   | O     | 460 | VAL  |
| 2   | N     | 402 | VAL  |
| 2   | O     | 392 | GLY  |
| 2   | O     | 658 | ILE  |
| 2   | N     | 658 | ILE  |

### 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     | 548/543 (101%)   | 525 (96%)  | 23 (4%)   | 26          | 25 |
| 1   | B     | 547/543 (101%)   | 524 (96%)  | 23 (4%)   | 26          | 25 |
| 1   | C     | 542/543 (100%)   | 519 (96%)  | 23 (4%)   | 26          | 25 |
| 1   | D     | 544/543 (100%)   | 520 (96%)  | 24 (4%)   | 25          | 23 |
| 2   | M     | 615/611 (101%)   | 566 (92%)  | 49 (8%)   | 11          | 7  |
| 2   | N     | 615/611 (101%)   | 571 (93%)  | 44 (7%)   | 13          | 8  |
| 2   | O     | 611/611 (100%)   | 510 (84%)  | 101 (16%) | 2           | 1  |
| 2   | P     | 611/611 (100%)   | 547 (90%)  | 64 (10%)  | 6           | 3  |
| All | All   | 4633/4616 (100%) | 4282 (92%) | 351 (8%)  | 12          | 8  |

All (351) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 27     | ARG  |
| 1   | A     | 140    | GLU  |
| 1   | A     | 153    | GLU  |
| 1   | A     | 159    | VAL  |
| 1   | A     | 206    | PHE  |
| 1   | A     | 284    | ASN  |
| 1   | A     | 298    | MET  |
| 1   | A     | 303    | LYS  |
| 1   | A     | 318    | THR  |
| 1   | A     | 415    | ASN  |
| 1   | A     | 418    | VAL  |
| 1   | A     | 426    | ARG  |
| 1   | A     | 427    | VAL  |
| 1   | A     | 438    | LYS  |
| 1   | A     | 466    | LEU  |
| 1   | A     | 482    | LEU  |
| 1   | A     | 518    | THR  |
| 1   | A     | 538    | GLU  |
| 1   | A     | 647    | ASP  |
| 1   | A     | 656    | LEU  |
| 1   | A     | 664    | GLU  |
| 1   | A     | 665[A] | ARG  |
| 1   | A     | 665[B] | ARG  |
| 1   | B     | 66     | ILE  |
| 1   | B     | 77     | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | B     | 120    | ILE  |
| 1   | B     | 148[A] | ARG  |
| 1   | B     | 148[B] | ARG  |
| 1   | B     | 153    | GLU  |
| 1   | B     | 159    | VAL  |
| 1   | B     | 206    | PHE  |
| 1   | B     | 308    | LYS  |
| 1   | B     | 318    | THR  |
| 1   | B     | 389    | GLN  |
| 1   | B     | 395    | GLU  |
| 1   | B     | 411    | ARG  |
| 1   | B     | 413    | GLU  |
| 1   | B     | 447    | ASN  |
| 1   | B     | 466    | LEU  |
| 1   | B     | 467    | ILE  |
| 1   | B     | 482    | LEU  |
| 1   | B     | 518    | THR  |
| 1   | B     | 537    | ILE  |
| 1   | B     | 600    | VAL  |
| 1   | B     | 647    | ASP  |
| 1   | B     | 656    | LEU  |
| 1   | C     | 23     | LYS  |
| 1   | C     | 27     | ARG  |
| 1   | C     | 81     | THR  |
| 1   | C     | 82     | ASP  |
| 1   | C     | 153    | GLU  |
| 1   | C     | 159    | VAL  |
| 1   | C     | 206    | PHE  |
| 1   | C     | 318    | THR  |
| 1   | C     | 323    | LEU  |
| 1   | C     | 359    | SER  |
| 1   | C     | 390    | THR  |
| 1   | C     | 395    | GLU  |
| 1   | C     | 418    | VAL  |
| 1   | C     | 466    | LEU  |
| 1   | C     | 467    | ILE  |
| 1   | C     | 482    | LEU  |
| 1   | C     | 539    | ILE  |
| 1   | C     | 600    | VAL  |
| 1   | C     | 639    | GLN  |
| 1   | C     | 647    | ASP  |
| 1   | C     | 656    | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 664  | GLU  |
| 1   | C     | 669  | LYS  |
| 1   | D     | 45   | VAL  |
| 1   | D     | 66   | ILE  |
| 1   | D     | 153  | GLU  |
| 1   | D     | 159  | VAL  |
| 1   | D     | 190  | ILE  |
| 1   | D     | 196  | GLU  |
| 1   | D     | 199  | ARG  |
| 1   | D     | 206  | PHE  |
| 1   | D     | 284  | ASN  |
| 1   | D     | 291  | ILE  |
| 1   | D     | 293  | GLN  |
| 1   | D     | 298  | MET  |
| 1   | D     | 299  | GLU  |
| 1   | D     | 331  | VAL  |
| 1   | D     | 413  | GLU  |
| 1   | D     | 423  | ILE  |
| 1   | D     | 427  | VAL  |
| 1   | D     | 466  | LEU  |
| 1   | D     | 467  | ILE  |
| 1   | D     | 470  | CYS  |
| 1   | D     | 594  | TRP  |
| 1   | D     | 600  | VAL  |
| 1   | D     | 656  | LEU  |
| 1   | D     | 664  | GLU  |
| 2   | M     | 6[A] | LYS  |
| 2   | M     | 6[B] | LYS  |
| 2   | M     | 14   | GLU  |
| 2   | M     | 66   | ARG  |
| 2   | M     | 125  | GLU  |
| 2   | M     | 169  | LEU  |
| 2   | M     | 198  | VAL  |
| 2   | M     | 199  | LYS  |
| 2   | M     | 214  | GLN  |
| 2   | M     | 215  | ILE  |
| 2   | M     | 245  | ARG  |
| 2   | M     | 249  | ARG  |
| 2   | M     | 262  | LYS  |
| 2   | M     | 314  | THR  |
| 2   | M     | 315  | LYS  |
| 2   | M     | 316  | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | M     | 317    | LYS  |
| 2   | M     | 318    | LEU  |
| 2   | M     | 332    | SER  |
| 2   | M     | 335    | LYS  |
| 2   | M     | 342    | MET  |
| 2   | M     | 354    | ARG  |
| 2   | M     | 373    | ILE  |
| 2   | M     | 376    | ILE  |
| 2   | M     | 380    | SER  |
| 2   | M     | 409    | ASP  |
| 2   | M     | 422    | GLN  |
| 2   | M     | 424    | ASN  |
| 2   | M     | 426    | ASN  |
| 2   | M     | 448    | LEU  |
| 2   | M     | 469    | THR  |
| 2   | M     | 475    | LYS  |
| 2   | M     | 486    | LYS  |
| 2   | M     | 539    | SER  |
| 2   | M     | 565    | LYS  |
| 2   | M     | 571    | LEU  |
| 2   | M     | 604    | ILE  |
| 2   | M     | 607    | GLU  |
| 2   | M     | 654    | SER  |
| 2   | M     | 672    | LYS  |
| 2   | M     | 674    | LEU  |
| 2   | M     | 681[A] | GLU  |
| 2   | M     | 681[B] | GLU  |
| 2   | M     | 684    | ARG  |
| 2   | M     | 694    | ASP  |
| 2   | M     | 702    | GLU  |
| 2   | M     | 704    | ILE  |
| 2   | M     | 724    | THR  |
| 2   | M     | 726    | ASP  |
| 2   | N     | 6      | LYS  |
| 2   | N     | 66     | ARG  |
| 2   | N     | 124    | ASP  |
| 2   | N     | 125    | GLU  |
| 2   | N     | 146    | ILE  |
| 2   | N     | 152    | THR  |
| 2   | N     | 174[A] | LYS  |
| 2   | N     | 174[B] | LYS  |
| 2   | N     | 198    | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 205 | ILE  |
| 2   | N     | 245 | ARG  |
| 2   | N     | 249 | ARG  |
| 2   | N     | 312 | LYS  |
| 2   | N     | 313 | LEU  |
| 2   | N     | 315 | LYS  |
| 2   | N     | 316 | ILE  |
| 2   | N     | 331 | GLU  |
| 2   | N     | 335 | LYS  |
| 2   | N     | 338 | MET  |
| 2   | N     | 354 | ARG  |
| 2   | N     | 358 | GLU  |
| 2   | N     | 373 | ILE  |
| 2   | N     | 386 | ILE  |
| 2   | N     | 388 | VAL  |
| 2   | N     | 405 | ARG  |
| 2   | N     | 424 | ASN  |
| 2   | N     | 425 | ILE  |
| 2   | N     | 440 | ARG  |
| 2   | N     | 448 | LEU  |
| 2   | N     | 471 | GLU  |
| 2   | N     | 492 | MET  |
| 2   | N     | 495 | LEU  |
| 2   | N     | 560 | ILE  |
| 2   | N     | 571 | LEU  |
| 2   | N     | 604 | ILE  |
| 2   | N     | 606 | PRO  |
| 2   | N     | 631 | LEU  |
| 2   | N     | 635 | ILE  |
| 2   | N     | 640 | GLN  |
| 2   | N     | 674 | LEU  |
| 2   | N     | 681 | GLU  |
| 2   | N     | 686 | SER  |
| 2   | N     | 693 | GLU  |
| 2   | N     | 702 | GLU  |
| 2   | O     | 6   | LYS  |
| 2   | O     | 17  | GLU  |
| 2   | O     | 39  | LEU  |
| 2   | O     | 64  | VAL  |
| 2   | O     | 66  | ARG  |
| 2   | O     | 71  | GLU  |
| 2   | O     | 95  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 125 | GLU  |
| 2   | O     | 127 | LEU  |
| 2   | O     | 149 | VAL  |
| 2   | O     | 152 | THR  |
| 2   | O     | 166 | SER  |
| 2   | O     | 169 | LEU  |
| 2   | O     | 174 | LYS  |
| 2   | O     | 185 | ILE  |
| 2   | O     | 198 | VAL  |
| 2   | O     | 205 | ILE  |
| 2   | O     | 214 | GLN  |
| 2   | O     | 216 | VAL  |
| 2   | O     | 233 | THR  |
| 2   | O     | 238 | GLU  |
| 2   | O     | 245 | ARG  |
| 2   | O     | 246 | ARG  |
| 2   | O     | 313 | LEU  |
| 2   | O     | 314 | THR  |
| 2   | O     | 315 | LYS  |
| 2   | O     | 316 | ILE  |
| 2   | O     | 317 | LYS  |
| 2   | O     | 318 | LEU  |
| 2   | O     | 322 | ILE  |
| 2   | O     | 333 | ILE  |
| 2   | O     | 335 | LYS  |
| 2   | O     | 339 | TYR  |
| 2   | O     | 342 | MET  |
| 2   | O     | 350 | PHE  |
| 2   | O     | 351 | GLU  |
| 2   | O     | 352 | LEU  |
| 2   | O     | 366 | ILE  |
| 2   | O     | 367 | GLU  |
| 2   | O     | 368 | VAL  |
| 2   | O     | 376 | ILE  |
| 2   | O     | 391 | TYR  |
| 2   | O     | 395 | MET  |
| 2   | O     | 404 | GLU  |
| 2   | O     | 407 | ILE  |
| 2   | O     | 411 | ILE  |
| 2   | O     | 426 | ASN  |
| 2   | O     | 427 | TRP  |
| 2   | O     | 428 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 429 | ARG  |
| 2   | O     | 432 | LYS  |
| 2   | O     | 448 | LEU  |
| 2   | O     | 449 | VAL  |
| 2   | O     | 453 | LYS  |
| 2   | O     | 454 | GLU  |
| 2   | O     | 459 | ILE  |
| 2   | O     | 463 | VAL  |
| 2   | O     | 467 | ILE  |
| 2   | O     | 478 | MET  |
| 2   | O     | 480 | VAL  |
| 2   | O     | 482 | ARG  |
| 2   | O     | 484 | LYS  |
| 2   | O     | 487 | GLU  |
| 2   | O     | 488 | ARG  |
| 2   | O     | 491 | ARG  |
| 2   | O     | 492 | MET  |
| 2   | O     | 493 | ARG  |
| 2   | O     | 495 | LEU  |
| 2   | O     | 497 | ASP  |
| 2   | O     | 499 | THR  |
| 2   | O     | 500 | VAL  |
| 2   | O     | 502 | THR  |
| 2   | O     | 511 | SER  |
| 2   | O     | 524 | ARG  |
| 2   | O     | 541 | GLU  |
| 2   | O     | 542 | ILE  |
| 2   | O     | 556 | GLU  |
| 2   | O     | 567 | VAL  |
| 2   | O     | 573 | THR  |
| 2   | O     | 575 | SER  |
| 2   | O     | 579 | LEU  |
| 2   | O     | 580 | GLU  |
| 2   | O     | 592 | MET  |
| 2   | O     | 608 | CYS  |
| 2   | O     | 612 | MET  |
| 2   | O     | 621 | MET  |
| 2   | O     | 631 | LEU  |
| 2   | O     | 641 | THR  |
| 2   | O     | 647 | ILE  |
| 2   | O     | 659 | SER  |
| 2   | O     | 672 | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 683 | VAL  |
| 2   | O     | 686 | SER  |
| 2   | O     | 687 | VAL  |
| 2   | O     | 691 | LEU  |
| 2   | O     | 693 | GLU  |
| 2   | O     | 696 | ILE  |
| 2   | O     | 697 | ASP  |
| 2   | O     | 708 | VAL  |
| 2   | O     | 723 | LEU  |
| 2   | O     | 729 | MET  |
| 2   | P     | 39  | LEU  |
| 2   | P     | 64  | VAL  |
| 2   | P     | 66  | ARG  |
| 2   | P     | 120 | LYS  |
| 2   | P     | 124 | ASP  |
| 2   | P     | 125 | GLU  |
| 2   | P     | 152 | THR  |
| 2   | P     | 166 | SER  |
| 2   | P     | 174 | LYS  |
| 2   | P     | 175 | GLU  |
| 2   | P     | 198 | VAL  |
| 2   | P     | 199 | LYS  |
| 2   | P     | 205 | ILE  |
| 2   | P     | 238 | GLU  |
| 2   | P     | 245 | ARG  |
| 2   | P     | 284 | GLU  |
| 2   | P     | 300 | LYS  |
| 2   | P     | 301 | ILE  |
| 2   | P     | 312 | LYS  |
| 2   | P     | 317 | LYS  |
| 2   | P     | 331 | GLU  |
| 2   | P     | 332 | SER  |
| 2   | P     | 335 | LYS  |
| 2   | P     | 341 | GLU  |
| 2   | P     | 342 | MET  |
| 2   | P     | 346 | ARG  |
| 2   | P     | 347 | THR  |
| 2   | P     | 351 | GLU  |
| 2   | P     | 354 | ARG  |
| 2   | P     | 362 | THR  |
| 2   | P     | 369 | ILE  |
| 2   | P     | 373 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 394 | LYS  |
| 2   | P     | 398 | ASP  |
| 2   | P     | 403 | LEU  |
| 2   | P     | 404 | GLU  |
| 2   | P     | 422 | GLN  |
| 2   | P     | 424 | ASN  |
| 2   | P     | 428 | LEU  |
| 2   | P     | 442 | LYS  |
| 2   | P     | 448 | LEU  |
| 2   | P     | 462 | ARG  |
| 2   | P     | 467 | ILE  |
| 2   | P     | 469 | THR  |
| 2   | P     | 480 | VAL  |
| 2   | P     | 482 | ARG  |
| 2   | P     | 483 | GLU  |
| 2   | P     | 486 | LYS  |
| 2   | P     | 500 | VAL  |
| 2   | P     | 502 | THR  |
| 2   | P     | 537 | LYS  |
| 2   | P     | 541 | GLU  |
| 2   | P     | 542 | ILE  |
| 2   | P     | 549 | GLN  |
| 2   | P     | 553 | LYS  |
| 2   | P     | 557 | ILE  |
| 2   | P     | 581 | GLN  |
| 2   | P     | 605 | LEU  |
| 2   | P     | 631 | LEU  |
| 2   | P     | 674 | LEU  |
| 2   | P     | 686 | SER  |
| 2   | P     | 717 | GLU  |
| 2   | P     | 726 | ASP  |
| 2   | P     | 729 | MET  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 122 | HIS  |
| 1   | A     | 164 | GLN  |
| 1   | A     | 201 | HIS  |
| 1   | A     | 209 | HIS  |
| 1   | A     | 217 | ASN  |
| 1   | A     | 218 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 220 | HIS  |
| 1   | A     | 284 | ASN  |
| 1   | A     | 471 | ASN  |
| 1   | A     | 477 | GLN  |
| 1   | A     | 479 | ASN  |
| 1   | A     | 503 | GLN  |
| 1   | A     | 515 | ASN  |
| 1   | B     | 9   | HIS  |
| 1   | B     | 122 | HIS  |
| 1   | B     | 201 | HIS  |
| 1   | B     | 209 | HIS  |
| 1   | B     | 217 | ASN  |
| 1   | B     | 218 | GLN  |
| 1   | B     | 220 | HIS  |
| 1   | B     | 260 | GLN  |
| 1   | B     | 275 | GLN  |
| 1   | B     | 293 | GLN  |
| 1   | B     | 454 | GLN  |
| 1   | B     | 477 | GLN  |
| 1   | B     | 565 | ASN  |
| 1   | B     | 672 | GLN  |
| 1   | C     | 9   | HIS  |
| 1   | C     | 201 | HIS  |
| 1   | C     | 209 | HIS  |
| 1   | C     | 217 | ASN  |
| 1   | C     | 218 | GLN  |
| 1   | C     | 220 | HIS  |
| 1   | C     | 275 | GLN  |
| 1   | C     | 368 | HIS  |
| 1   | C     | 454 | GLN  |
| 1   | C     | 477 | GLN  |
| 1   | C     | 503 | GLN  |
| 1   | C     | 515 | ASN  |
| 1   | C     | 622 | GLN  |
| 1   | C     | 639 | GLN  |
| 1   | C     | 672 | GLN  |
| 1   | D     | 201 | HIS  |
| 1   | D     | 209 | HIS  |
| 1   | D     | 217 | ASN  |
| 1   | D     | 218 | GLN  |
| 1   | D     | 220 | HIS  |
| 1   | D     | 284 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 293 | GLN  |
| 1   | D     | 477 | GLN  |
| 1   | D     | 622 | GLN  |
| 1   | D     | 639 | GLN  |
| 2   | M     | 211 | ASN  |
| 2   | M     | 287 | GLN  |
| 2   | M     | 375 | GLN  |
| 2   | M     | 408 | HIS  |
| 2   | M     | 424 | ASN  |
| 2   | M     | 426 | ASN  |
| 2   | M     | 544 | HIS  |
| 2   | M     | 581 | GLN  |
| 2   | M     | 590 | ASN  |
| 2   | N     | 211 | ASN  |
| 2   | N     | 345 | ASN  |
| 2   | N     | 396 | GLN  |
| 2   | N     | 408 | HIS  |
| 2   | N     | 424 | ASN  |
| 2   | N     | 510 | GLN  |
| 2   | N     | 581 | GLN  |
| 2   | N     | 590 | ASN  |
| 2   | N     | 640 | GLN  |
| 2   | O     | 27  | HIS  |
| 2   | O     | 95  | ASN  |
| 2   | O     | 211 | ASN  |
| 2   | O     | 244 | GLN  |
| 2   | O     | 419 | HIS  |
| 2   | O     | 515 | ASN  |
| 2   | O     | 516 | HIS  |
| 2   | O     | 568 | ASN  |
| 2   | O     | 576 | ASN  |
| 2   | O     | 590 | ASN  |
| 2   | O     | 618 | HIS  |
| 2   | O     | 640 | GLN  |
| 2   | P     | 27  | HIS  |
| 2   | P     | 211 | ASN  |
| 2   | P     | 287 | GLN  |
| 2   | P     | 396 | GLN  |
| 2   | P     | 408 | HIS  |
| 2   | P     | 422 | GLN  |
| 2   | P     | 424 | ASN  |
| 2   | P     | 426 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 443 | ASN  |
| 2   | P     | 516 | HIS  |
| 2   | P     | 549 | GLN  |
| 2   | P     | 578 | ASN  |
| 2   | P     | 581 | GLN  |
| 2   | P     | 590 | ASN  |

### 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 34 ligands modelled in this entry, 12 are monoatomic - leaving 22 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | XCC  | C     | 800 | 10,1 | 0,11,11      | -    | -           | -           |      |             |
| 3   | SF4  | P     | 900 | 2    | 0,12,12      | -    | -           | -           |      |             |
| 3   | SF4  | C     | 700 | 1    | 0,12,12      | -    | -           | -           |      |             |
| 4   | XCC  | A     | 800 | 10,1 | 0,11,11      | -    | -           | -           |      |             |
| 5   | GOL  | A     | 863 | -    | 5,5,5        | 0.45 | 0           | 5,5,5       | 1.82 | 2 (40%)     |
| 5   | GOL  | B     | 863 | -    | 5,5,5        | 1.10 | 1 (20%)     | 5,5,5       | 1.85 | 1 (20%)     |
| 8   | ACT  | P     | 953 | -    | 1,2,3        | 1.54 | 0           | 0,1,3       | -    | -           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | ACT  | N     | 953 | -    | 1,2,3        | 1.45 | 0        | 0,1,3       | -    | -        |
| 3   | SF4  | M     | 900 | 2    | 0,12,12      | -    | -        | -           |      |          |
| 3   | SF4  | N     | 900 | 2    | 0,12,12      | -    | -        | -           |      |          |
| 4   | XCC  | B     | 800 | 10,1 | 0,11,11      | -    | -        | -           |      |          |
| 8   | ACT  | M     | 953 | -    | 1,2,3        | 1.35 | 0        | 0,1,3       | -    | -        |
| 3   | SF4  | A     | 700 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 3   | SF4  | D     | 750 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 8   | ACT  | O     | 953 | -    | 1,2,3        | 1.23 | 0        | 0,1,3       | -    | -        |
| 3   | SF4  | O     | 900 | 2    | 0,12,12      | -    | -        | -           |      |          |
| 3   | SF4  | A     | 750 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 4   | XCC  | D     | 800 | 10,1 | 0,11,11      | -    | -        | -           |      |          |
| 3   | SF4  | B     | 750 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 5   | GOL  | C     | 863 | -    | 5,5,5        | 0.31 | 0        | 5,5,5       | 0.65 | 0        |
| 3   | SF4  | C     | 750 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 5   | GOL  | D     | 863 | -    | 5,5,5        | 0.54 | 0        | 5,5,5       | 1.72 | 2 (40%)  |

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 |
| 5   | GOL  | C     | 863 | -    | -       | 2/4/4/4  | -       |
| 5   | GOL  | A     | 863 | -    | -       | 2/4/4/4  | -       |
| 3   | SF4  | B     | 750 | 1    | -       | -        | 0/6/5/5 |
| 3   | SF4  | O     | 900 | 2    | -       | -        | 0/6/5/5 |
| 3   | SF4  | P     | 900 | 2    | -       | -        | 0/6/5/5 |
| 3   | SF4  | C     | 700 | 1    | -       | -        | 0/6/5/5 |
| 4   | XCC  | C     | 800 | 10,1 | -       | -        | 0/3/3/3 |
| 3   | SF4  | A     | 750 | 1    | -       | -        | 0/6/5/5 |
| 3   | SF4  | C     | 750 | 1    | -       | -        | 0/6/5/5 |
| 4   | XCC  | B     | 800 | 10,1 | -       | -        | 0/3/3/3 |
| 5   | GOL  | B     | 863 | -    | -       | 0/4/4/4  | -       |
| 4   | XCC  | A     | 800 | 10,1 | -       | -        | 0/3/3/3 |
| 3   | SF4  | A     | 700 | 1    | -       | -        | 0/6/5/5 |
| 4   | XCC  | D     | 800 | 10,1 | -       | -        | 0/3/3/3 |
| 3   | SF4  | D     | 750 | 1    | -       | -        | 0/6/5/5 |
| 5   | GOL  | D     | 863 | -    | -       | 3/4/4/4  | -       |
| 3   | SF4  | M     | 900 | 2    | -       | -        | 0/6/5/5 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | B     | 863 | GOL  | O2-C2 | -2.41 | 1.36        | 1.43     |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | B     | 863 | GOL  | O2-C2-C3 | -3.29 | 95.57       | 109.18   |
| 5   | D     | 863 | GOL  | O1-C1-C2 | -2.87 | 97.45       | 110.38   |
| 5   | A     | 863 | GOL  | O1-C1-C2 | -2.49 | 99.16       | 110.38   |
| 5   | A     | 863 | GOL  | O3-C3-C2 | -2.06 | 101.10      | 110.38   |
| 5   | D     | 863 | GOL  | O2-C2-C1 | -2.01 | 100.86      | 109.18   |

There are no chirality outliers.

All (7) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 5   | A     | 863 | GOL  | O1-C1-C2-C3 |
| 5   | C     | 863 | GOL  | O1-C1-C2-C3 |
| 5   | D     | 863 | GOL  | O1-C1-C2-C3 |
| 5   | C     | 863 | GOL  | O1-C1-C2-O2 |
| 5   | D     | 863 | GOL  | O1-C1-C2-O2 |
| 5   | A     | 863 | GOL  | O1-C1-C2-O2 |
| 5   | D     | 863 | GOL  | O2-C2-C3-O3 |

There are no ring outliers.

10 monomers are involved in 21 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | C     | 700 | SF4  | 1       | 0            |
| 4   | A     | 800 | XCC  | 1       | 0            |
| 8   | P     | 953 | ACT  | 1       | 0            |
| 3   | N     | 900 | SF4  | 1       | 0            |
| 8   | O     | 953 | ACT  | 1       | 0            |
| 3   | O     | 900 | SF4  | 2       | 0            |
| 4   | D     | 800 | XCC  | 2       | 0            |
| 3   | B     | 750 | SF4  | 1       | 0            |
| 5   | C     | 863 | GOL  | 5       | 0            |
| 5   | D     | 863 | GOL  | 6       | 0            |

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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%)   | -0.26  | 2 (0%)    | 90 | 91 | 14, 25, 43, 60        | 7 (1%)  |
| 1   | B     | 673/674 (99%)   | -0.39  | 8 (1%)    | 76 | 79 | 11, 22, 39, 68        | 5 (0%)  |
| 1   | C     | 673/674 (99%)   | -0.17  | 1 (0%)    | 92 | 93 | 15, 28, 42, 58        | 2 (0%)  |
| 1   | D     | 673/674 (99%)   | -0.01  | 3 (0%)    | 88 | 90 | 13, 31, 45, 59        | 4 (0%)  |
| 2   | M     | 728/729 (99%)   | 0.18   | 23 (3%)   | 50 | 54 | 12, 33, 62, 74        | 5 (0%)  |
| 2   | N     | 728/729 (99%)   | 0.22   | 57 (7%)   | 19 | 21 | 10, 32, 66, 76        | 6 (0%)  |
| 2   | O     | 728/729 (99%)   | 1.61   | 261 (35%) | 1  | 1  | 26, 64, 92, 126       | 1 (0%)  |
| 2   | P     | 728/729 (99%)   | 0.66   | 84 (11%)  | 9  | 10 | 15, 45, 76, 92        | 1 (0%)  |
| All | All   | 5604/5612 (99%) | 0.25   | 439 (7%)  | 19 | 21 | 10, 31, 74, 126       | 31 (0%) |

All (439) RSRZ outliers are listed below:

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 2   | O     | 312[A] | LYS  | 6.6  |
| 2   | O     | 728    | ILE  | 6.4  |
| 2   | O     | 458    | ALA  | 5.9  |
| 2   | O     | 428    | LEU  | 5.9  |
| 2   | O     | 495    | LEU  | 5.8  |
| 2   | O     | 683    | VAL  | 5.5  |
| 2   | O     | 397    | ALA  | 5.5  |
| 2   | O     | 480    | VAL  | 5.3  |
| 2   | O     | 691    | LEU  | 5.3  |
| 2   | O     | 457    | PRO  | 5.2  |
| 2   | O     | 647    | ILE  | 5.2  |
| 2   | O     | 366    | ILE  | 5.2  |
| 2   | O     | 481    | ALA  | 5.0  |
| 1   | B     | 539    | ILE  | 5.0  |
| 2   | O     | 574    | ALA  | 5.0  |
| 2   | O     | 353    | VAL  | 5.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 2   | O     | 567    | VAL  | 5.0  |
| 2   | O     | 449    | VAL  | 4.8  |
| 2   | O     | 474    | VAL  | 4.8  |
| 2   | O     | 316    | ILE  | 4.8  |
| 2   | O     | 339    | TYR  | 4.7  |
| 2   | N     | 480    | VAL  | 4.7  |
| 2   | O     | 344    | GLY  | 4.7  |
| 2   | N     | 486[A] | LYS  | 4.6  |
| 2   | O     | 425    | ILE  | 4.6  |
| 2   | O     | 472    | ALA  | 4.5  |
| 2   | O     | 369    | ILE  | 4.5  |
| 2   | O     | 724    | THR  | 4.5  |
| 2   | O     | 463    | VAL  | 4.5  |
| 2   | O     | 450    | ALA  | 4.5  |
| 2   | O     | 368    | VAL  | 4.4  |
| 2   | O     | 488    | ARG  | 4.4  |
| 2   | O     | 542    | ILE  | 4.4  |
| 2   | O     | 361    | ILE  | 4.3  |
| 2   | O     | 340    | VAL  | 4.2  |
| 2   | O     | 348    | PRO  | 4.2  |
| 2   | O     | 477    | TYR  | 4.2  |
| 2   | O     | 570    | TYR  | 4.2  |
| 2   | N     | 468    | PHE  | 4.2  |
| 2   | O     | 399    | PHE  | 4.2  |
| 2   | O     | 467    | ILE  | 4.2  |
| 2   | O     | 356    | VAL  | 4.2  |
| 2   | O     | 460    | VAL  | 4.2  |
| 2   | O     | 525    | VAL  | 4.2  |
| 2   | O     | 427    | TRP  | 4.2  |
| 2   | O     | 485    | TYR  | 4.1  |
| 2   | O     | 465    | VAL  | 4.1  |
| 2   | O     | 579    | LEU  | 4.1  |
| 2   | O     | 552    | PRO  | 4.1  |
| 2   | O     | 355    | THR  | 4.1  |
| 2   | O     | 377    | PRO  | 4.0  |
| 2   | O     | 382    | LEU  | 4.0  |
| 1   | B     | 416    | ARG  | 4.0  |
| 2   | O     | 350    | PHE  | 4.0  |
| 2   | O     | 708    | VAL  | 4.0  |
| 2   | O     | 352    | LEU  | 3.9  |
| 2   | O     | 534    | LEU  | 3.9  |
| 2   | O     | 687    | VAL  | 3.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | N     | 348 | PRO  | 3.9  |
| 2   | O     | 468 | PHE  | 3.9  |
| 1   | A     | 415 | ASN  | 3.9  |
| 2   | P     | 356 | VAL  | 3.8  |
| 2   | O     | 722 | ALA  | 3.8  |
| 2   | O     | 402 | VAL  | 3.8  |
| 2   | O     | 484 | LYS  | 3.8  |
| 2   | O     | 545 | ALA  | 3.8  |
| 2   | P     | 495 | LEU  | 3.8  |
| 2   | O     | 494 | GLY  | 3.8  |
| 2   | O     | 469 | THR  | 3.7  |
| 2   | O     | 380 | SER  | 3.7  |
| 2   | O     | 723 | LEU  | 3.7  |
| 2   | N     | 481 | ALA  | 3.7  |
| 2   | O     | 700 | ALA  | 3.7  |
| 2   | O     | 383 | PRO  | 3.7  |
| 2   | N     | 729 | MET  | 3.7  |
| 2   | O     | 459 | ILE  | 3.7  |
| 2   | O     | 595 | CYS  | 3.6  |
| 2   | O     | 388 | VAL  | 3.6  |
| 2   | O     | 390 | ILE  | 3.6  |
| 2   | O     | 560 | ILE  | 3.6  |
| 2   | O     | 593 | THR  | 3.6  |
| 2   | N     | 474 | VAL  | 3.6  |
| 2   | O     | 531 | VAL  | 3.6  |
| 2   | P     | 474 | VAL  | 3.6  |
| 2   | O     | 557 | ILE  | 3.6  |
| 2   | O     | 486 | LYS  | 3.6  |
| 2   | M     | 316 | ILE  | 3.6  |
| 2   | O     | 587 | LEU  | 3.6  |
| 2   | O     | 482 | ARG  | 3.6  |
| 2   | O     | 526 | GLY  | 3.6  |
| 2   | O     | 322 | ILE  | 3.5  |
| 2   | O     | 386 | ILE  | 3.5  |
| 2   | O     | 551 | ILE  | 3.5  |
| 2   | P     | 728 | ILE  | 3.5  |
| 2   | N     | 387 | LEU  | 3.5  |
| 2   | O     | 417 | LEU  | 3.5  |
| 2   | O     | 471 | GLU  | 3.5  |
| 2   | P     | 425 | ILE  | 3.5  |
| 2   | O     | 364 | GLY  | 3.5  |
| 2   | M     | 314 | THR  | 3.5  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 2   | M     | 640[A] | GLN  | 3.5  |
| 2   | O     | 373    | ILE  | 3.5  |
| 2   | O     | 519    | ILE  | 3.5  |
| 2   | O     | 665    | ALA  | 3.5  |
| 2   | O     | 540    | TYR  | 3.5  |
| 2   | O     | 473    | LYS  | 3.5  |
| 2   | P     | 353    | VAL  | 3.5  |
| 2   | O     | 314    | THR  | 3.5  |
| 2   | P     | 316    | ILE  | 3.4  |
| 2   | O     | 407    | ILE  | 3.4  |
| 2   | O     | 362    | THR  | 3.4  |
| 2   | N     | 316    | ILE  | 3.4  |
| 2   | O     | 639    | THR  | 3.3  |
| 2   | P     | 496    | THR  | 3.3  |
| 2   | O     | 572    | TYR  | 3.3  |
| 2   | O     | 559    | PRO  | 3.3  |
| 2   | O     | 696    | ILE  | 3.3  |
| 2   | P     | 350    | PHE  | 3.3  |
| 2   | O     | 563    | ILE  | 3.3  |
| 2   | O     | 667    | ILE  | 3.3  |
| 2   | M     | 318    | LEU  | 3.3  |
| 2   | N     | 318    | LEU  | 3.3  |
| 2   | O     | 387    | LEU  | 3.3  |
| 2   | O     | 470    | ASP  | 3.3  |
| 2   | O     | 496    | THR  | 3.3  |
| 2   | O     | 544    | HIS  | 3.3  |
| 2   | O     | 376    | ILE  | 3.3  |
| 2   | P     | 428    | LEU  | 3.3  |
| 2   | O     | 645    | MET  | 3.3  |
| 2   | P     | 729    | MET  | 3.3  |
| 2   | O     | 389    | ASP  | 3.3  |
| 2   | O     | 547    | PRO  | 3.2  |
| 2   | M     | 458    | ALA  | 3.2  |
| 2   | N     | 361    | ILE  | 3.2  |
| 2   | O     | 699    | ILE  | 3.2  |
| 2   | O     | 384    | LEU  | 3.2  |
| 2   | N     | 650    | THR  | 3.2  |
| 2   | O     | 686    | SER  | 3.2  |
| 2   | O     | 478    | MET  | 3.2  |
| 2   | O     | 492    | MET  | 3.2  |
| 2   | O     | 394    | LYS  | 3.2  |
| 2   | O     | 504    | TYR  | 3.2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | P     | 639 | THR  | 3.2  |
| 2   | N     | 315 | LYS  | 3.2  |
| 2   | O     | 442 | LYS  | 3.2  |
| 2   | O     | 655 | LYS  | 3.2  |
| 2   | O     | 729 | MET  | 3.2  |
| 2   | O     | 714 | TYR  | 3.2  |
| 2   | O     | 711 | ILE  | 3.1  |
| 2   | O     | 664 | ILE  | 3.1  |
| 2   | O     | 347 | THR  | 3.1  |
| 2   | O     | 420 | THR  | 3.1  |
| 2   | O     | 456 | PHE  | 3.1  |
| 2   | O     | 682 | PHE  | 3.1  |
| 2   | O     | 430 | VAL  | 3.1  |
| 1   | B     | 537 | ILE  | 3.1  |
| 2   | P     | 336 | GLY  | 3.1  |
| 2   | O     | 713 | PRO  | 3.1  |
| 2   | P     | 486 | LYS  | 3.1  |
| 2   | O     | 678 | LEU  | 3.1  |
| 2   | O     | 564 | TRP  | 3.0  |
| 2   | O     | 444 | TYR  | 3.0  |
| 2   | O     | 491 | ARG  | 3.0  |
| 2   | P     | 481 | ALA  | 3.0  |
| 2   | O     | 447 | ILE  | 3.0  |
| 2   | P     | 333 | ILE  | 3.0  |
| 2   | O     | 346 | ARG  | 3.0  |
| 2   | O     | 663 | GLY  | 3.0  |
| 2   | M     | 729 | MET  | 3.0  |
| 2   | O     | 395 | MET  | 3.0  |
| 2   | O     | 333 | ILE  | 3.0  |
| 2   | O     | 707 | THR  | 3.0  |
| 1   | D     | 417 | PRO  | 3.0  |
| 2   | O     | 371 | PRO  | 3.0  |
| 2   | P     | 559 | PRO  | 3.0  |
| 2   | O     | 451 | LYS  | 3.0  |
| 2   | O     | 421 | GLY  | 3.0  |
| 2   | P     | 339 | TYR  | 3.0  |
| 2   | O     | 594 | SER  | 2.9  |
| 2   | O     | 345 | ASN  | 2.9  |
| 2   | P     | 579 | LEU  | 2.9  |
| 2   | N     | 638 | GLY  | 2.9  |
| 2   | O     | 553 | LYS  | 2.9  |
| 2   | N     | 362 | THR  | 2.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | O     | 670 | MET  | 2.9  |
| 2   | O     | 436 | ALA  | 2.9  |
| 2   | O     | 583 | CYS  | 2.9  |
| 2   | O     | 650 | THR  | 2.9  |
| 2   | N     | 383 | PRO  | 2.9  |
| 2   | O     | 317 | LYS  | 2.9  |
| 2   | N     | 472 | ALA  | 2.9  |
| 2   | O     | 712 | LEU  | 2.9  |
| 2   | O     | 601 | ILE  | 2.9  |
| 2   | O     | 613 | ILE  | 2.9  |
| 2   | O     | 391 | TYR  | 2.9  |
| 2   | P     | 683 | VAL  | 2.8  |
| 2   | P     | 355 | THR  | 2.8  |
| 2   | N     | 390 | ILE  | 2.8  |
| 2   | O     | 475 | LYS  | 2.8  |
| 2   | O     | 503 | PHE  | 2.8  |
| 2   | P     | 418 | TRP  | 2.8  |
| 2   | O     | 641 | THR  | 2.8  |
| 2   | N     | 376 | ILE  | 2.8  |
| 2   | N     | 360 | GLU  | 2.8  |
| 2   | N     | 434 | ALA  | 2.8  |
| 2   | M     | 382 | LEU  | 2.8  |
| 2   | O     | 466 | THR  | 2.8  |
| 2   | O     | 573 | THR  | 2.8  |
| 2   | O     | 653 | VAL  | 2.8  |
| 2   | O     | 721 | PRO  | 2.8  |
| 2   | P     | 427 | TRP  | 2.8  |
| 2   | P     | 623 | PRO  | 2.8  |
| 2   | O     | 431 | SER  | 2.8  |
| 2   | N     | 466 | THR  | 2.8  |
| 2   | O     | 586 | THR  | 2.8  |
| 2   | M     | 728 | ILE  | 2.8  |
| 2   | N     | 366 | ILE  | 2.8  |
| 2   | O     | 354 | ARG  | 2.7  |
| 2   | O     | 441 | PHE  | 2.7  |
| 2   | P     | 477 | TYR  | 2.7  |
| 2   | P     | 584 | LEU  | 2.7  |
| 2   | O     | 500 | VAL  | 2.7  |
| 2   | O     | 418 | TRP  | 2.7  |
| 2   | O     | 497 | ASP  | 2.7  |
| 2   | O     | 637 | GLY  | 2.7  |
| 2   | O     | 365 | LYS  | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 2   | P     | 660    | ALA  | 2.7  |
| 2   | O     | 403    | LEU  | 2.7  |
| 1   | B     | 443    | GLN  | 2.7  |
| 2   | N     | 369    | ILE  | 2.7  |
| 2   | O     | 715    | LEU  | 2.7  |
| 2   | P     | 320    | LEU  | 2.7  |
| 2   | P     | 715    | LEU  | 2.7  |
| 2   | O     | 623    | PRO  | 2.7  |
| 2   | O     | 652    | ILE  | 2.7  |
| 2   | P     | 369    | ILE  | 2.7  |
| 2   | N     | 545    | ALA  | 2.6  |
| 2   | O     | 499    | THR  | 2.6  |
| 2   | O     | 657    | PHE  | 2.6  |
| 2   | M     | 345    | ASN  | 2.6  |
| 2   | N     | 384    | LEU  | 2.6  |
| 2   | P     | 552    | PRO  | 2.6  |
| 2   | N     | 300[A] | LYS  | 2.6  |
| 2   | N     | 368    | VAL  | 2.6  |
| 2   | O     | 435    | VAL  | 2.6  |
| 2   | O     | 507    | VAL  | 2.6  |
| 2   | P     | 583    | CYS  | 2.6  |
| 2   | M     | 481    | ALA  | 2.6  |
| 2   | N     | 458    | ALA  | 2.6  |
| 2   | P     | 700    | ALA  | 2.6  |
| 2   | M     | 313    | LEU  | 2.6  |
| 2   | O     | 401    | GLY  | 2.6  |
| 2   | O     | 662    | GLY  | 2.6  |
| 2   | P     | 492    | MET  | 2.6  |
| 2   | O     | 426    | ASN  | 2.6  |
| 2   | O     | 632    | ALA  | 2.6  |
| 2   | N     | 495    | LEU  | 2.6  |
| 2   | O     | 396    | GLN  | 2.6  |
| 2   | P     | 407    | ILE  | 2.6  |
| 2   | O     | 336    | GLY  | 2.6  |
| 2   | P     | 478    | MET  | 2.6  |
| 2   | O     | 381    | LYS  | 2.6  |
| 2   | P     | 475    | LYS  | 2.6  |
| 2   | P     | 484    | LYS  | 2.6  |
| 2   | O     | 434    | ALA  | 2.6  |
| 2   | O     | 359    | SER  | 2.6  |
| 2   | O     | 571    | LEU  | 2.6  |
| 2   | P     | 712    | LEU  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | M     | 376 | ILE  | 2.5  |
| 2   | N     | 728 | ILE  | 2.5  |
| 2   | O     | 611 | ILE  | 2.5  |
| 2   | O     | 668 | VAL  | 2.5  |
| 2   | N     | 370 | GLY  | 2.5  |
| 2   | O     | 648 | GLY  | 2.5  |
| 2   | O     | 530 | ALA  | 2.5  |
| 2   | O     | 606 | PRO  | 2.5  |
| 2   | N     | 350 | PHE  | 2.5  |
| 2   | O     | 695 | PHE  | 2.5  |
| 2   | N     | 373 | ILE  | 2.5  |
| 2   | N     | 388 | VAL  | 2.5  |
| 2   | O     | 627 | THR  | 2.5  |
| 2   | O     | 619 | ALA  | 2.5  |
| 2   | O     | 674 | LEU  | 2.5  |
| 2   | P     | 387 | LEU  | 2.5  |
| 2   | O     | 533 | TRP  | 2.5  |
| 2   | N     | 317 | LYS  | 2.5  |
| 2   | N     | 463 | VAL  | 2.5  |
| 2   | M     | 124 | ASP  | 2.5  |
| 2   | M     | 693 | GLU  | 2.5  |
| 2   | N     | 367 | GLU  | 2.5  |
| 2   | O     | 566 | SER  | 2.5  |
| 2   | M     | 371 | PRO  | 2.5  |
| 2   | O     | 612 | MET  | 2.5  |
| 1   | D     | 368 | HIS  | 2.5  |
| 2   | O     | 335 | LYS  | 2.5  |
| 2   | P     | 335 | LYS  | 2.5  |
| 2   | M     | 467 | ILE  | 2.5  |
| 2   | N     | 467 | ILE  | 2.5  |
| 2   | P     | 359 | SER  | 2.4  |
| 2   | P     | 362 | THR  | 2.4  |
| 2   | O     | 318 | LEU  | 2.4  |
| 2   | O     | 605 | LEU  | 2.4  |
| 2   | M     | 343 | GLY  | 2.4  |
| 2   | O     | 385 | GLY  | 2.4  |
| 2   | O     | 638 | GLY  | 2.4  |
| 2   | O     | 520 | VAL  | 2.4  |
| 2   | O     | 704 | ILE  | 2.4  |
| 2   | O     | 669 | TRP  | 2.4  |
| 2   | N     | 377 | PRO  | 2.4  |
| 2   | O     | 602 | MET  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 2   | P     | 488    | ARG  | 2.4  |
| 2   | P     | 491    | ARG  | 2.4  |
| 1   | B     | 536    | ASN  | 2.4  |
| 2   | O     | 582    | VAL  | 2.4  |
| 2   | P     | 460    | VAL  | 2.4  |
| 2   | O     | 634    | MET  | 2.4  |
| 1   | D     | 669[A] | LYS  | 2.4  |
| 2   | O     | 502    | THR  | 2.4  |
| 2   | P     | 482    | ARG  | 2.4  |
| 2   | P     | 713    | PRO  | 2.4  |
| 2   | P     | 727    | PRO  | 2.4  |
| 1   | B     | 538    | GLU  | 2.4  |
| 2   | O     | 476    | GLU  | 2.4  |
| 2   | O     | 562    | GLY  | 2.4  |
| 2   | O     | 719    | GLY  | 2.4  |
| 2   | P     | 555    | GLY  | 2.4  |
| 2   | O     | 229    | PHE  | 2.4  |
| 2   | O     | 635    | ILE  | 2.4  |
| 2   | P     | 340    | VAL  | 2.4  |
| 2   | P     | 480    | VAL  | 2.4  |
| 2   | P     | 493    | ARG  | 2.4  |
| 1   | A     | 368    | HIS  | 2.4  |
| 2   | N     | 639    | THR  | 2.4  |
| 2   | P     | 485    | TYR  | 2.3  |
| 2   | M     | 472    | ALA  | 2.3  |
| 2   | O     | 689    | GLU  | 2.3  |
| 2   | N     | 313    | LEU  | 2.3  |
| 2   | O     | 448    | LEU  | 2.3  |
| 2   | O     | 392    | GLY  | 2.3  |
| 2   | P     | 373    | ILE  | 2.3  |
| 2   | P     | 402    | VAL  | 2.3  |
| 2   | N     | 485    | TYR  | 2.3  |
| 2   | N     | 382    | LEU  | 2.3  |
| 2   | O     | 313    | LEU  | 2.3  |
| 2   | P     | 313    | LEU  | 2.3  |
| 2   | P     | 723    | LEU  | 2.3  |
| 2   | N     | 124    | ASP  | 2.3  |
| 2   | O     | 124    | ASP  | 2.3  |
| 2   | N     | 492    | MET  | 2.3  |
| 2   | O     | 342    | MET  | 2.3  |
| 2   | P     | 361    | ILE  | 2.3  |
| 2   | N     | 371    | PRO  | 2.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | O     | 424 | ASN  | 2.3  |
| 2   | M     | 637 | GLY  | 2.3  |
| 2   | N     | 392 | GLY  | 2.3  |
| 2   | N     | 477 | TYR  | 2.3  |
| 2   | O     | 585 | TYR  | 2.3  |
| 2   | N     | 425 | ILE  | 2.3  |
| 2   | P     | 376 | ILE  | 2.3  |
| 2   | O     | 522 | PRO  | 2.3  |
| 2   | O     | 727 | PRO  | 2.3  |
| 2   | M     | 315 | LYS  | 2.3  |
| 2   | O     | 432 | LYS  | 2.3  |
| 2   | P     | 562 | GLY  | 2.3  |
| 2   | P     | 638 | GLY  | 2.3  |
| 2   | P     | 342 | MET  | 2.3  |
| 2   | O     | 151 | TRP  | 2.3  |
| 2   | O     | 679 | HIS  | 2.2  |
| 2   | O     | 410 | PHE  | 2.2  |
| 2   | P     | 459 | ILE  | 2.2  |
| 2   | P     | 377 | PRO  | 2.2  |
| 2   | O     | 538 | ALA  | 2.2  |
| 2   | P     | 397 | ALA  | 2.2  |
| 2   | N     | 391 | TYR  | 2.2  |
| 2   | O     | 13  | PRO  | 2.2  |
| 2   | O     | 604 | ILE  | 2.2  |
| 2   | O     | 642 | PRO  | 2.2  |
| 2   | P     | 420 | THR  | 2.2  |
| 2   | P     | 557 | ILE  | 2.2  |
| 2   | O     | 584 | LEU  | 2.2  |
| 2   | O     | 631 | LEU  | 2.2  |
| 2   | P     | 572 | TYR  | 2.2  |
| 2   | O     | 698 | LYS  | 2.2  |
| 2   | P     | 371 | PRO  | 2.2  |
| 2   | O     | 343 | GLY  | 2.2  |
| 2   | O     | 516 | HIS  | 2.2  |
| 2   | O     | 518 | CYS  | 2.2  |
| 2   | P     | 571 | LEU  | 2.2  |
| 2   | P     | 570 | TYR  | 2.2  |
| 2   | O     | 615 | THR  | 2.2  |
| 2   | O     | 716 | GLU  | 2.1  |
| 2   | P     | 483 | GLU  | 2.1  |
| 2   | O     | 517 | VAL  | 2.1  |
| 2   | O     | 506 | CYS  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | O     | 505 | SER  | 2.1  |
| 2   | M     | 477 | TYR  | 2.1  |
| 2   | O     | 558 | ASP  | 2.1  |
| 2   | O     | 614 | THR  | 2.1  |
| 2   | P     | 457 | PRO  | 2.1  |
| 2   | P     | 560 | ILE  | 2.1  |
| 2   | P     | 664 | ILE  | 2.1  |
| 2   | O     | 600 | ALA  | 2.1  |
| 2   | O     | 357 | SER  | 2.1  |
| 2   | N     | 469 | THR  | 2.1  |
| 2   | O     | 423 | ARG  | 2.1  |
| 2   | O     | 546 | GLY  | 2.1  |
| 2   | O     | 658 | ILE  | 2.1  |
| 2   | N     | 465 | VAL  | 2.1  |
| 2   | O     | 338 | MET  | 2.1  |
| 2   | O     | 725 | MET  | 2.1  |
| 2   | N     | 314 | THR  | 2.1  |
| 2   | P     | 385 | GLY  | 2.1  |
| 1   | C     | 539 | ILE  | 2.1  |
| 2   | M     | 390 | ILE  | 2.1  |
| 2   | O     | 146 | ILE  | 2.1  |
| 2   | O     | 512 | PHE  | 2.1  |
| 2   | P     | 533 | TRP  | 2.1  |
| 1   | B     | 155 | GLU  | 2.0  |
| 2   | O     | 532 | SER  | 2.1  |
| 2   | O     | 659 | SER  | 2.1  |
| 2   | O     | 452 | MET  | 2.0  |
| 2   | O     | 588 | MET  | 2.0  |
| 2   | P     | 403 | LEU  | 2.0  |
| 2   | O     | 576 | ASN  | 2.0  |
| 2   | N     | 389 | ASP  | 2.0  |
| 2   | P     | 501 | ASP  | 2.0  |
| 2   | O     | 493 | ARG  | 2.0  |
| 2   | M     | 724 | THR  | 2.0  |
| 2   | N     | 473 | LYS  | 2.0  |
| 2   | O     | 561 | LYS  | 2.0  |
| 2   | P     | 394 | LYS  | 2.0  |
| 2   | P     | 432 | LYS  | 2.0  |
| 1   | B     | 540 | GLY  | 2.0  |
| 2   | P     | 682 | PHE  | 2.0  |
| 2   | O     | 654 | SER  | 2.0  |
| 2   | P     | 357 | SER  | 2.0  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | N     | 490 | ASP  | 2.0  |
| 2   | O     | 694 | ASP  | 2.0  |
| 2   | O     | 651 | TYR  | 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 5   | GOL  | C     | 863 | 6/6   | 0.77 | 0.17 | 47,56,56,58                | 0     |
| 9   | NA   | O     | 730 | 1/1   | 0.86 | 0.10 | 70,70,70,70                | 0     |
| 5   | GOL  | D     | 863 | 6/6   | 0.87 | 0.13 | 43,46,48,48                | 0     |
| 9   | NA   | P     | 730 | 1/1   | 0.87 | 0.08 | 35,35,35,35                | 0     |
| 8   | ACT  | N     | 953 | 3/4   | 0.89 | 0.21 | 59,59,59,59                | 0     |
| 8   | ACT  | P     | 953 | 3/4   | 0.90 | 0.21 | 53,53,54,54                | 0     |
| 8   | ACT  | M     | 953 | 3/4   | 0.93 | 0.15 | 44,44,44,45                | 0     |
| 5   | GOL  | A     | 863 | 6/6   | 0.93 | 0.10 | 26,30,33,37                | 0     |
| 8   | ACT  | O     | 953 | 3/4   | 0.93 | 0.23 | 100,100,100,100            | 0     |
| 3   | SF4  | O     | 900 | 8/8   | 0.94 | 0.07 | 61,63,67,67                | 0     |
| 5   | GOL  | B     | 863 | 6/6   | 0.96 | 0.08 | 26,30,34,37                | 0     |
| 6   | CU1  | P     | 950 | 1/1   | 0.96 | 0.05 | 55,55,55,55                | 0     |
| 9   | NA   | M     | 730 | 1/1   | 0.97 | 0.05 | 29,29,29,29                | 0     |
| 9   | NA   | N     | 730 | 1/1   | 0.97 | 0.03 | 28,28,28,28                | 0     |
| 6   | CU1  | O     | 950 | 1/1   | 0.97 | 0.04 | 82,82,82,82                | 0     |
| 7   | NI   | O     | 951 | 1/1   | 0.97 | 0.06 | 76,76,76,76                | 0     |
| 3   | SF4  | C     | 700 | 8/8   | 0.98 | 0.04 | 28,32,35,35                | 0     |
| 3   | SF4  | P     | 900 | 8/8   | 0.98 | 0.04 | 40,40,41,46                | 0     |
| 4   | XCC  | C     | 800 | 9/9   | 0.98 | 0.04 | 25,27,34,35                | 0     |
| 6   | CU1  | N     | 950 | 1/1   | 0.99 | 0.04 | 38,38,38,38                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | SF4  | A     | 750 | 8/8   | 0.99 | 0.03 | 14,17,17,18                 | 0     |
| 3   | SF4  | B     | 750 | 8/8   | 0.99 | 0.03 | 17,18,18,19                 | 0     |
| 7   | NI   | M     | 951 | 1/1   | 0.99 | 0.02 | 28,28,28,28                 | 0     |
| 4   | XCC  | A     | 800 | 9/9   | 0.99 | 0.03 | 20,24,29,30                 | 0     |
| 7   | NI   | P     | 951 | 1/1   | 0.99 | 0.04 | 39,39,39,39                 | 0     |
| 4   | XCC  | B     | 800 | 9/9   | 0.99 | 0.03 | 16,20,25,27                 | 0     |
| 3   | SF4  | A     | 700 | 8/8   | 0.99 | 0.03 | 17,19,20,22                 | 0     |
| 4   | XCC  | D     | 800 | 9/9   | 0.99 | 0.03 | 33,35,41,45                 | 0     |
| 3   | SF4  | C     | 750 | 8/8   | 0.99 | 0.03 | 28,30,31,32                 | 0     |
| 3   | SF4  | D     | 750 | 8/8   | 0.99 | 0.05 | 26,28,29,29                 | 0     |
| 3   | SF4  | M     | 900 | 8/8   | 0.99 | 0.03 | 22,25,26,28                 | 0     |
| 3   | SF4  | N     | 900 | 8/8   | 0.99 | 0.03 | 25,26,27,28                 | 0     |
| 6   | CU1  | M     | 950 | 1/1   | 0.99 | 0.03 | 43,43,43,43                 | 0     |
| 7   | NI   | N     | 951 | 1/1   | 1.00 | 0.01 | 29,29,29,29                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.