



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:28 PM GMT

PDB ID : 1KEK  
Title : Crystal Structure of the Free Radical Intermediate of Pyruvate:Ferredoxin Oxidoreductase  
Authors : Chabriere, E.; Vernede, X.; Guigliarelli, B.; Charon, M.-H.; Hatchikian, E.C.; Fontecilla-Camps, J.C.  
Deposited on : 2001-11-16  
Resolution : 1.90 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

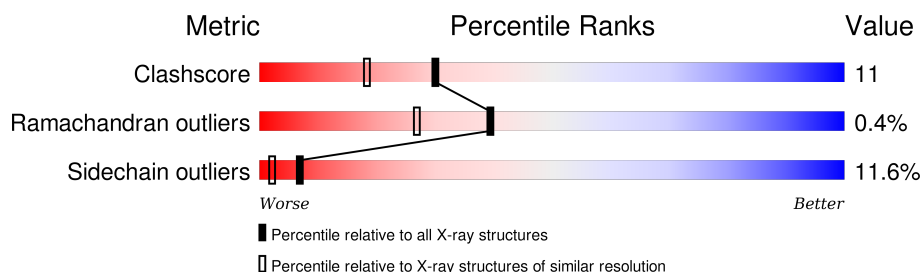
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 102246                      | 5398 (1.90-1.90)                                      |
| Ramachandran outliers | 100387                      | 5338 (1.90-1.90)                                      |
| Sidechain outliers    | 100360                      | 5339 (1.90-1.90)                                      |

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1231   | <br>70% 23% 5% • |
| 1   | B     | 1231   | <br>73% 21% • •  |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20775 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 Pyruvate-Ferredoxin Oxidoreductase.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1231     | Total | C    | N    | O    | S  | 36      | 0       | 0     |
|     |       |          | 9383  | 5941 | 1599 | 1784 | 59 |         |         |       |
| 1   | B     | 1231     | Total | C    | N    | O    | S  | 41      | 0       | 0     |
|     |       |          | 9383  | 5941 | 1599 | 1784 | 59 |         |         |       |

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | B     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

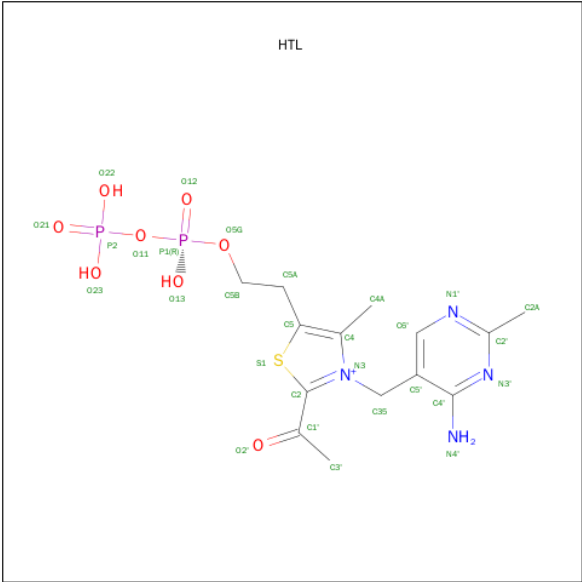
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | B     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | A     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



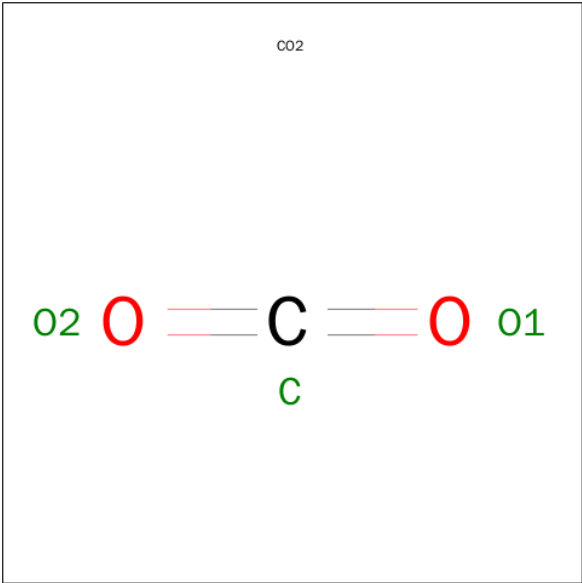
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 4   | A     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 4   | A     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 4   | A     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 4   | B     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 4   | B     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 4   | B     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |

- Molecule 5 is 2-ACETYL-THIAMINE DIPHOSPHATE (three-letter code: HTL) (formula:  $C_{14}H_{21}N_4O_8P_2S$ ).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |   |
|-----|-------|----------|-------|----|---|---|---|---------|---------|---|
| 5   | A     | 1        | Total | C  | N | O | P | S       | 0       | 0 |
|     |       |          | 29    | 14 | 4 | 8 | 2 | 1       |         |   |
| 5   | B     | 1        | Total | C  | N | O | P | S       | 0       | 0 |
|     |       |          | 29    | 14 | 4 | 8 | 2 | 1       |         |   |

- Molecule 6 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO<sub>2</sub>).



| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 6   | A     | 1        | Total | C O | 0       | 0       |
|     |       |          | 3     | 1 2 |         |         |
| 6   | B     | 1        | Total | C O | 0       | 0       |
|     |       |          | 3     | 1 2 |         |         |

- Molecule 7 is water.

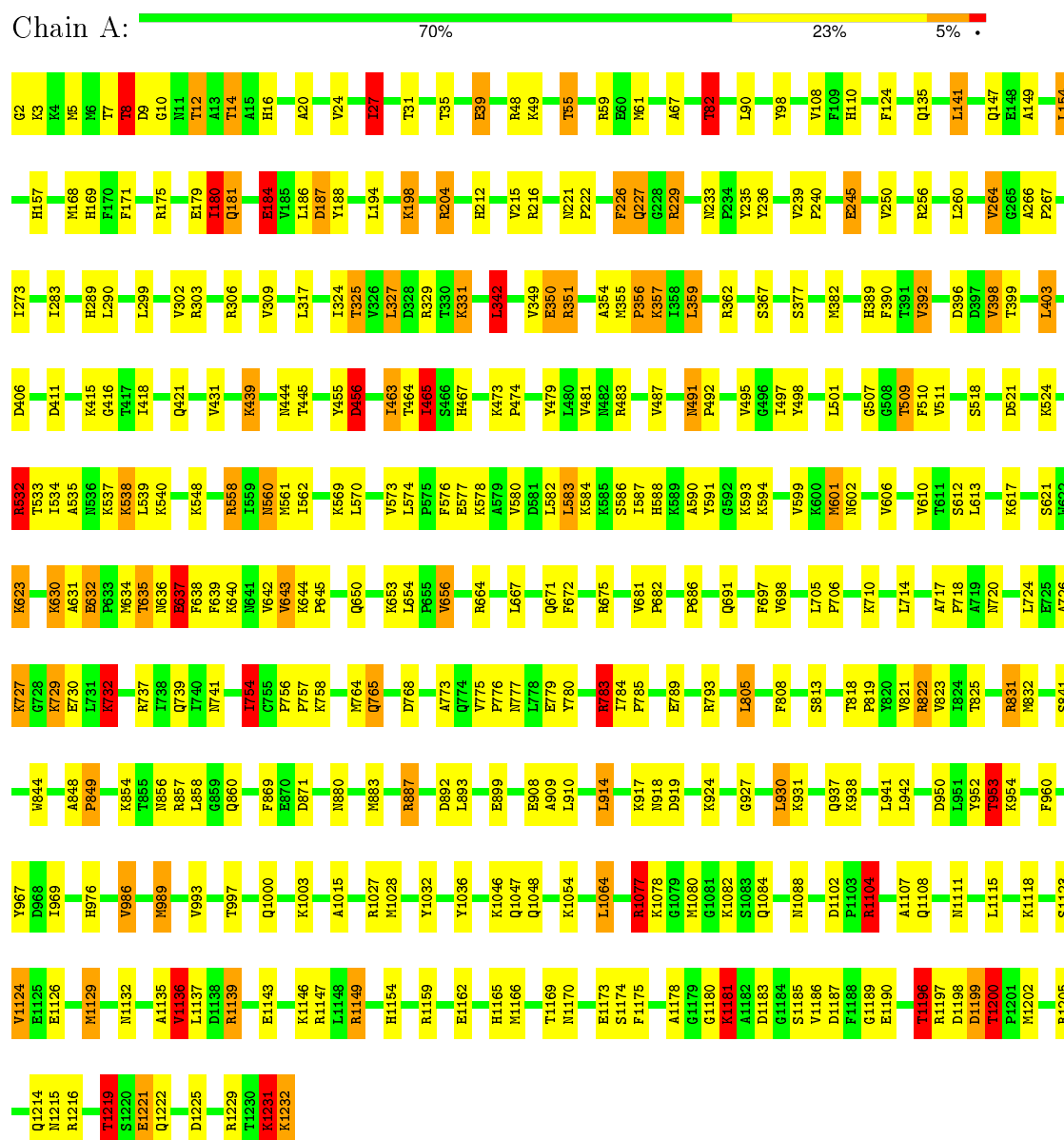
| Mol | Chain | Residues | Atoms         |           | ZeroOcc | AltConf |
|-----|-------|----------|---------------|-----------|---------|---------|
| 7   | A     | 851      | Total<br>851  | O<br>851  | 0       | 0       |
| 7   | B     | 1042     | Total<br>1042 | O<br>1042 | 0       | 0       |

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

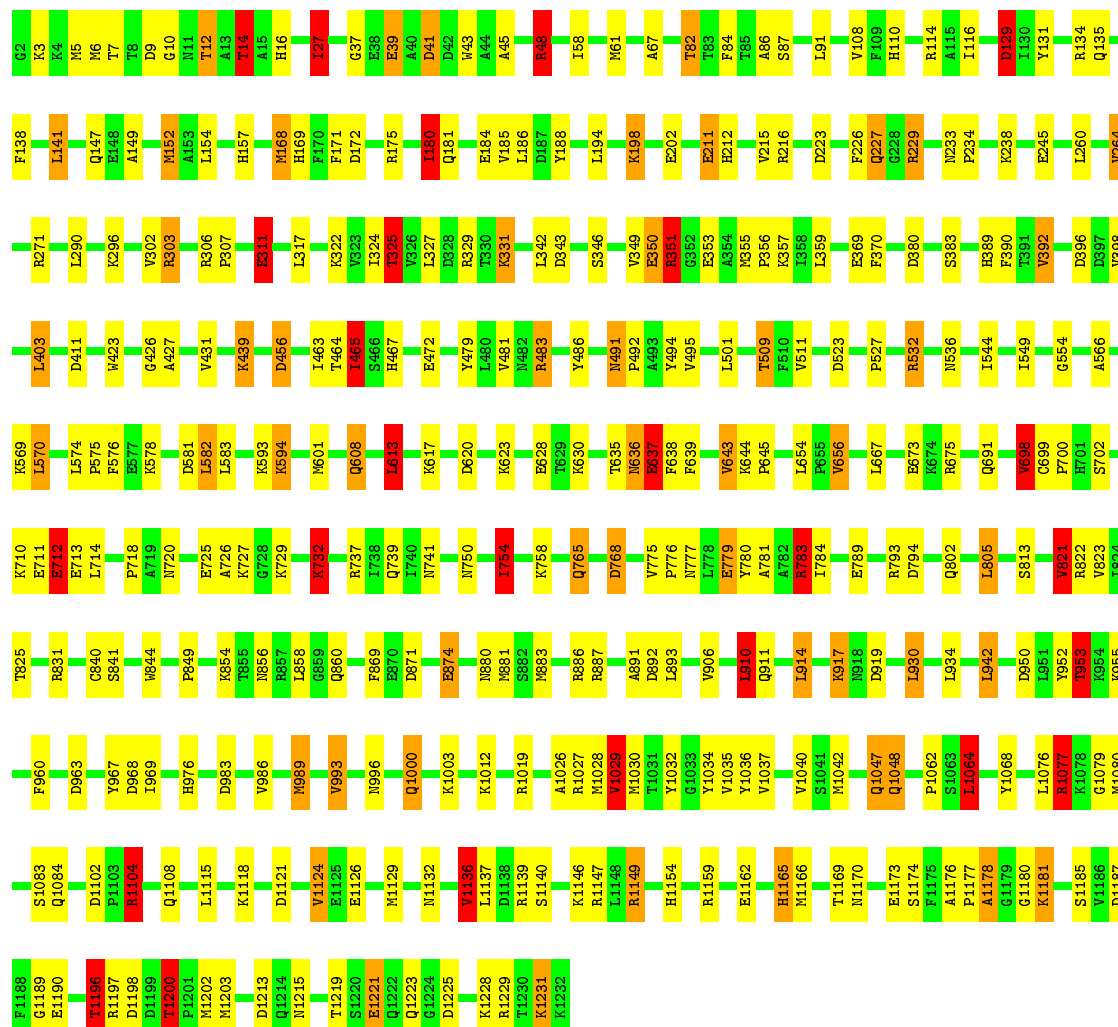
Note EDS was not executed.

#### • Molecule 1: Pyruvate-Ferredoxin Oxidoreductase



• Molecule 1: Pyruvate-Ferredoxin Oxidoreductase

Chain B: 73% 21% • •





## 4 Data and refinement statistics

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

| Property   | Value   | Source    |
|--|---|-----------|
| Space group  | P 21 21 21  | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 86.11 Å   145.76 Å   210.26 Å<br>90.00°   90.00°   90.00° | Depositor |
| Resolution (Å)   | 27.38 – 1.90  | Depositor |
| % Data completeness<br>(in resolution range)             | 97.5 (27.38-1.90)   | Depositor |
| $R_{merge}$  | (Not available)   | Depositor |
| $R_{sym}$  | 0.08  | Depositor |
| Refinement program                                       | X-PLOR, REFMAC  | Depositor |
| R, $R_{free}$  | 0.178 , 0.227   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                                    | Xtriage   |
| Total number of atoms                                    | 20775   | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 28.0  | wwPDB-VP  |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CO2, CA, SF4, HTL

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     | 0.78         | 10/9585 (0.1%)  | 1.56        | 147/12954 (1.1%) |
| 1   | B     | 1.07         | 14/9585 (0.1%)  | 1.63        | 154/12954 (1.2%) |
| All | All   | 0.94         | 24/19170 (0.1%) | 1.60        | 301/25908 (1.2%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 1   | B     | 2                   | 3                   |
| All | All   | 2                   | 5                   |

All (24) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1   | B     | 732  | LYS  | CD-CE | 56.96  | 2.93        | 1.51     |
| 1   | B     | 1231 | LYS  | C-N   | 28.83  | 2.00        | 1.34     |
| 1   | B     | 732  | LYS  | CG-CD | -20.40 | 0.83        | 1.52     |
| 1   | A     | 601  | MET  | C-O   | -15.37 | 0.94        | 1.23     |
| 1   | B     | 711  | GLU  | C-O   | -15.06 | 0.94        | 1.23     |
| 1   | A     | 601  | MET  | CA-CB | -14.13 | 1.22        | 1.53     |
| 1   | A     | 601  | MET  | CA-C  | 14.07  | 1.89        | 1.52     |
| 1   | B     | 712  | GLU  | C-O   | -13.72 | 0.97        | 1.23     |
| 1   | B     | 711  | GLU  | CA-CB | -12.56 | 1.26        | 1.53     |
| 1   | A     | 532  | ARG  | CA-C  | 11.83  | 1.83        | 1.52     |
| 1   | B     | 732  | LYS  | CA-CB | -10.97 | 1.29        | 1.53     |
| 1   | B     | 712  | GLU  | CA-C  | 10.27  | 1.79        | 1.52     |
| 1   | A     | 1147 | ARG  | CG-CD | 9.54   | 1.75        | 1.51     |
| 1   | B     | 712  | GLU  | CA-CB | -9.17  | 1.33        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 908  | GLU  | CB-CG  | -9.12 | 1.34        | 1.52     |
| 1   | B     | 1126 | GLU  | C-O    | -9.12 | 1.06        | 1.23     |
| 1   | A     | 532  | ARG  | CA-CB  | -7.74 | 1.36        | 1.53     |
| 1   | B     | 711  | GLU  | CA-C   | 7.53  | 1.72        | 1.52     |
| 1   | B     | 48   | ARG  | CD-NE  | -7.51 | 1.33        | 1.46     |
| 1   | A     | 637  | GLU  | CA-CB  | 5.64  | 1.66        | 1.53     |
| 1   | A     | 532  | ARG  | C-N    | -5.56 | 1.21        | 1.34     |
| 1   | A     | 540  | LYS  | CD-CE  | -5.39 | 1.37        | 1.51     |
| 1   | B     | 245  | GLU  | C-O    | -5.22 | 1.13        | 1.23     |
| 1   | B     | 637  | GLU  | CD-OE2 | 5.10  | 1.31        | 1.25     |

All (301) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1   | B     | 532  | ARG  | CD-NE-CZ  | 35.55  | 173.37      | 123.60   |
| 1   | B     | 48   | ARG  | CD-NE-CZ  | 30.27  | 165.97      | 123.60   |
| 1   | A     | 204  | ARG  | CD-NE-CZ  | 29.99  | 165.58      | 123.60   |
| 1   | A     | 48   | ARG  | NE-CZ-NH2 | -21.39 | 109.60      | 120.30   |
| 1   | A     | 351  | ARG  | NE-CZ-NH1 | 21.10  | 130.85      | 120.30   |
| 1   | B     | 732  | LYS  | CG-CD-CE  | -20.30 | 51.01       | 111.90   |
| 1   | A     | 601  | MET  | O-C-N     | 19.00  | 153.10      | 122.70   |
| 1   | A     | 351  | ARG  | NE-CZ-NH2 | -17.44 | 111.58      | 120.30   |
| 1   | B     | 732  | LYS  | N-CA-CB   | 17.03  | 141.25      | 110.60   |
| 1   | A     | 204  | ARG  | NE-CZ-NH1 | -15.41 | 112.59      | 120.30   |
| 1   | B     | 1077 | ARG  | NE-CZ-NH2 | -14.85 | 112.88      | 120.30   |
| 1   | B     | 48   | ARG  | CG-CD-NE  | 14.70  | 142.67      | 111.80   |
| 1   | A     | 48   | ARG  | CD-NE-CZ  | 14.58  | 144.01      | 123.60   |
| 1   | B     | 351  | ARG  | NE-CZ-NH1 | 14.43  | 127.52      | 120.30   |
| 1   | B     | 306  | ARG  | NE-CZ-NH1 | 14.22  | 127.41      | 120.30   |
| 1   | B     | 48   | ARG  | NE-CZ-NH2 | -14.07 | 113.26      | 120.30   |
| 1   | B     | 712  | GLU  | N-CA-CB   | 13.68  | 135.22      | 110.60   |
| 1   | A     | 601  | MET  | N-CA-CB   | 13.55  | 135.00      | 110.60   |
| 1   | B     | 1231 | LYS  | CA-C-N    | -13.40 | 87.72       | 117.20   |
| 1   | A     | 664  | ARG  | NE-CZ-NH2 | -13.20 | 113.70      | 120.30   |
| 1   | A     | 1205 | ARG  | NE-CZ-NH1 | -12.02 | 114.29      | 120.30   |
| 1   | B     | 822  | ARG  | NE-CZ-NH1 | -11.73 | 114.43      | 120.30   |
| 1   | B     | 1147 | ARG  | NE-CZ-NH1 | 11.64  | 126.12      | 120.30   |
| 1   | B     | 355  | MET  | CA-CB-CG  | 11.64  | 133.09      | 113.30   |
| 1   | A     | 1104 | ARG  | NE-CZ-NH2 | 11.58  | 126.09      | 120.30   |
| 1   | A     | 532  | ARG  | O-C-N     | 11.37  | 140.90      | 122.70   |
| 1   | B     | 793  | ARG  | NE-CZ-NH2 | -11.21 | 114.69      | 120.30   |
| 1   | A     | 1104 | ARG  | NE-CZ-NH1 | -11.17 | 114.71      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 1   | B     | 48   | ARG  | NH1-CZ-NH2 | 11.05  | 131.55      | 119.40   |
| 1   | A     | 1200 | THR  | N-CA-CB    | -10.95 | 89.49       | 110.30   |
| 1   | A     | 216  | ARG  | CD-NE-CZ   | 10.89  | 138.85      | 123.60   |
| 1   | B     | 1159 | ARG  | NE-CZ-NH1  | 10.80  | 125.70      | 120.30   |
| 1   | B     | 1104 | ARG  | CD-NE-CZ   | 10.79  | 138.71      | 123.60   |
| 1   | A     | 783  | ARG  | NE-CZ-NH1  | 10.78  | 125.69      | 120.30   |
| 1   | B     | 712  | GLU  | O-C-N      | 10.65  | 139.75      | 122.70   |
| 1   | A     | 887  | ARG  | NE-CZ-NH2  | 10.54  | 125.57      | 120.30   |
| 1   | A     | 832  | MET  | CA-CB-CG   | 10.32  | 130.84      | 113.30   |
| 1   | B     | 48   | ARG  | NE-CZ-NH1  | -10.28 | 115.16      | 120.30   |
| 1   | A     | 351  | ARG  | CD-NE-CZ   | 10.27  | 137.98      | 123.60   |
| 1   | B     | 675  | ARG  | NE-CZ-NH2  | -10.16 | 115.22      | 120.30   |
| 1   | A     | 919  | ASP  | CB-CG-OD1  | 9.88   | 127.19      | 118.30   |
| 1   | B     | 351  | ARG  | NE-CZ-NH2  | -9.75  | 115.43      | 120.30   |
| 1   | A     | 601  | MET  | CA-C-N     | -9.69  | 95.88       | 117.20   |
| 1   | A     | 1149 | ARG  | NE-CZ-NH2  | -9.67  | 115.46      | 120.30   |
| 1   | B     | 456  | ASP  | CB-CG-OD1  | 9.67   | 127.00      | 118.30   |
| 1   | A     | 1205 | ARG  | NE-CZ-NH2  | 9.64   | 125.12      | 120.30   |
| 1   | A     | 1104 | ARG  | CD-NE-CZ   | 9.61   | 137.05      | 123.60   |
| 1   | A     | 675  | ARG  | NE-CZ-NH1  | 9.41   | 125.00      | 120.30   |
| 1   | B     | 675  | ARG  | NE-CZ-NH1  | 9.31   | 124.95      | 120.30   |
| 1   | B     | 380  | ASP  | CB-CG-OD1  | 9.23   | 126.61      | 118.30   |
| 1   | A     | 675  | ARG  | NE-CZ-NH2  | -9.20  | 115.70      | 120.30   |
| 1   | B     | 711  | GLU  | N-CA-CB    | 9.13   | 127.03      | 110.60   |
| 1   | B     | 532  | ARG  | NE-CZ-NH1  | 9.11   | 124.86      | 120.30   |
| 1   | A     | 48   | ARG  | NH1-CZ-NH2 | 8.93   | 129.23      | 119.40   |
| 1   | B     | 822  | ARG  | NE-CZ-NH2  | 8.93   | 124.77      | 120.30   |
| 1   | B     | 1136 | VAL  | CB-CA-C    | -8.90  | 94.48       | 111.40   |
| 1   | A     | 27   | ILE  | CA-CB-CG2  | 8.84   | 128.57      | 110.90   |
| 1   | B     | 1032 | TYR  | CB-CG-CD2  | 8.83   | 126.30      | 121.00   |
| 1   | B     | 172  | ASP  | CB-CG-OD2  | 8.81   | 126.23      | 118.30   |
| 1   | A     | 1136 | VAL  | CB-CA-C    | -8.73  | 94.82       | 111.40   |
| 1   | A     | 908  | GLU  | CA-CB-CG   | 8.71   | 132.55      | 113.40   |
| 1   | A     | 675  | ARG  | CD-NE-CZ   | 8.66   | 135.72      | 123.60   |
| 1   | A     | 306  | ARG  | NE-CZ-NH1  | 8.47   | 124.54      | 120.30   |
| 1   | A     | 1124 | VAL  | CB-CA-C    | -8.46  | 95.32       | 111.40   |
| 1   | A     | 1196 | THR  | N-CA-CB    | -8.36  | 94.41       | 110.30   |
| 1   | B     | 216  | ARG  | NE-CZ-NH2  | -8.36  | 116.12      | 120.30   |
| 1   | A     | 39   | GLU  | OE1-CD-OE2 | 8.34   | 133.30      | 123.30   |
| 1   | B     | 131  | TYR  | CB-CG-CD1  | -8.31  | 116.01      | 121.00   |
| 1   | A     | 1219 | THR  | N-CA-CB    | -8.30  | 94.53       | 110.30   |
| 1   | B     | 392  | VAL  | CB-CA-C    | -8.27  | 95.68       | 111.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 455  | TYR  | CB-CG-CD2  | -8.18 | 116.09      | 121.00   |
| 1   | B     | 1221 | GLU  | CA-CB-CG   | 8.17  | 131.38      | 113.40   |
| 1   | B     | 1036 | TYR  | CB-CG-CD1  | 8.15  | 125.89      | 121.00   |
| 1   | B     | 82   | THR  | CB-CA-C    | -8.11 | 89.71       | 111.60   |
| 1   | A     | 532  | ARG  | CA-C-O     | -8.11 | 103.08      | 120.10   |
| 1   | B     | 989  | MET  | CG-SD-CE   | -8.04 | 87.33       | 100.20   |
| 1   | B     | 712  | GLU  | CA-C-N     | -7.98 | 99.64       | 117.20   |
| 1   | B     | 732  | LYS  | CB-CA-C    | -7.96 | 94.49       | 110.40   |
| 1   | B     | 27   | ILE  | CA-CB-CG2  | 7.94  | 126.78      | 110.90   |
| 1   | B     | 711  | GLU  | CA-C-N     | -7.93 | 99.76       | 117.20   |
| 1   | B     | 675  | ARG  | CD-NE-CZ   | 7.84  | 134.57      | 123.60   |
| 1   | B     | 711  | GLU  | O-C-N      | 7.82  | 135.21      | 122.70   |
| 1   | B     | 343  | ASP  | CB-CG-OD2  | -7.76 | 111.31      | 118.30   |
| 1   | B     | 175  | ARG  | NE-CZ-NH1  | -7.75 | 116.42      | 120.30   |
| 1   | A     | 256  | ARG  | NE-CZ-NH2  | -7.70 | 116.45      | 120.30   |
| 1   | B     | 1126 | GLU  | N-CA-CB    | 7.67  | 124.40      | 110.60   |
| 1   | B     | 1200 | THR  | N-CA-CB    | -7.66 | 95.75       | 110.30   |
| 1   | A     | 783  | ARG  | NE-CZ-NH2  | -7.57 | 116.52      | 120.30   |
| 1   | B     | 369  | GLU  | OE1-CD-OE2 | 7.55  | 132.36      | 123.30   |
| 1   | A     | 8    | THR  | N-CA-CB    | 7.54  | 124.62      | 110.30   |
| 1   | B     | 698  | VAL  | N-CA-CB    | -7.54 | 94.92       | 111.50   |
| 1   | A     | 392  | VAL  | CB-CA-C    | -7.53 | 97.10       | 111.40   |
| 1   | B     | 1165 | HIS  | N-CA-CB    | 7.51  | 124.12      | 110.60   |
| 1   | A     | 1104 | ARG  | CG-CD-NE   | -7.48 | 96.09       | 111.80   |
| 1   | A     | 887  | ARG  | NE-CZ-NH1  | -7.40 | 116.60      | 120.30   |
| 1   | A     | 857  | ARG  | NE-CZ-NH1  | 7.38  | 123.99      | 120.30   |
| 1   | B     | 350  | GLU  | OE1-CD-OE2 | 7.34  | 132.11      | 123.30   |
| 1   | A     | 857  | ARG  | NE-CZ-NH2  | -7.31 | 116.64      | 120.30   |
| 1   | A     | 455  | TYR  | CB-CG-CD1  | 7.30  | 125.38      | 121.00   |
| 1   | B     | 952  | TYR  | CB-CG-CD1  | -7.27 | 116.64      | 121.00   |
| 1   | B     | 1196 | THR  | N-CA-CB    | -7.22 | 96.58       | 110.30   |
| 1   | A     | 1165 | HIS  | N-CA-CB    | 7.21  | 123.59      | 110.60   |
| 1   | B     | 1032 | TYR  | CB-CG-CD1  | -7.21 | 116.67      | 121.00   |
| 1   | B     | 114  | ARG  | NE-CZ-NH1  | 7.16  | 123.88      | 120.30   |
| 1   | A     | 180  | ILE  | CA-CB-CG2  | 7.14  | 125.17      | 110.90   |
| 1   | B     | 331  | LYS  | CD-CE-NZ   | -7.13 | 95.30       | 111.70   |
| 1   | A     | 479  | TYR  | CB-CG-CD1  | -7.12 | 116.73      | 121.00   |
| 1   | A     | 59   | ARG  | NE-CZ-NH2  | -7.11 | 116.74      | 120.30   |
| 1   | A     | 1129 | MET  | CG-SD-CE   | 7.10  | 111.57      | 100.20   |
| 1   | B     | 129  | ASP  | CB-CG-OD2  | 7.08  | 124.67      | 118.30   |
| 1   | A     | 187  | ASP  | CB-CG-OD2  | -7.08 | 111.93      | 118.30   |
| 1   | B     | 39   | GLU  | OE1-CD-OE2 | 7.05  | 131.76      | 123.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 331  | LYS  | CA-CB-CG   | 7.00  | 128.80      | 113.40   |
| 1   | B     | 41   | ASP  | CB-CG-OD1  | -7.00 | 112.00      | 118.30   |
| 1   | B     | 968  | ASP  | CB-CG-OD2  | 6.95  | 124.56      | 118.30   |
| 1   | A     | 82   | THR  | CB-CA-C    | -6.94 | 92.85       | 111.60   |
| 1   | B     | 1104 | ARG  | CG-CD-NE   | -6.91 | 97.28       | 111.80   |
| 1   | B     | 325  | THR  | N-CA-CB    | 6.90  | 123.41      | 110.30   |
| 1   | A     | 914  | LEU  | CA-CB-CG   | 6.89  | 131.14      | 115.30   |
| 1   | A     | 39   | GLU  | CG-CD-OE2  | -6.87 | 104.56      | 118.30   |
| 1   | A     | 264  | VAL  | CA-CB-CG1  | 6.79  | 121.08      | 110.90   |
| 1   | B     | 698  | VAL  | CG1-CB-CG2 | 6.78  | 121.75      | 110.90   |
| 1   | A     | 306  | ARG  | NE-CZ-NH2  | -6.73 | 116.94      | 120.30   |
| 1   | A     | 952  | TYR  | CB-CG-CD2  | 6.70  | 125.02      | 121.00   |
| 1   | A     | 39   | GLU  | CA-CB-CG   | -6.66 | 98.75       | 113.40   |
| 1   | A     | 637  | GLU  | CA-CB-CG   | 6.64  | 128.02      | 113.40   |
| 1   | B     | 306  | ARG  | NE-CZ-NH2  | -6.64 | 116.98      | 120.30   |
| 1   | A     | 1139 | ARG  | NE-CZ-NH2  | 6.64  | 123.62      | 120.30   |
| 1   | B     | 793  | ARG  | NE-CZ-NH1  | 6.63  | 123.61      | 120.30   |
| 1   | A     | 532  | ARG  | N-CA-CB    | 6.62  | 122.52      | 110.60   |
| 1   | B     | 523  | ASP  | CB-CG-OD2  | 6.58  | 124.22      | 118.30   |
| 1   | B     | 152  | MET  | CG-SD-CE   | -6.56 | 89.70       | 100.20   |
| 1   | B     | 1077 | ARG  | NE-CZ-NH1  | 6.52  | 123.56      | 120.30   |
| 1   | B     | 168  | MET  | CG-SD-CE   | 6.48  | 110.56      | 100.20   |
| 1   | A     | 302  | VAL  | CA-CB-CG2  | 6.47  | 120.61      | 110.90   |
| 1   | A     | 871  | ASP  | CB-CG-OD2  | 6.47  | 124.13      | 118.30   |
| 1   | B     | 783  | ARG  | NE-CZ-NH2  | 6.47  | 123.53      | 120.30   |
| 1   | B     | 370  | PHE  | CB-CG-CD1  | -6.45 | 116.29      | 120.80   |
| 1   | B     | 967  | TYR  | CB-CG-CD1  | 6.38  | 124.83      | 121.00   |
| 1   | B     | 914  | LEU  | CA-CB-CG   | 6.37  | 129.95      | 115.30   |
| 1   | B     | 823  | VAL  | CA-CB-CG2  | 6.37  | 120.45      | 110.90   |
| 1   | A     | 656  | VAL  | CA-CB-CG2  | 6.33  | 120.40      | 110.90   |
| 1   | A     | 1197 | ARG  | NE-CZ-NH2  | -6.32 | 117.14      | 120.30   |
| 1   | A     | 98   | TYR  | CB-CG-CD1  | -6.31 | 117.21      | 121.00   |
| 1   | A     | 793  | ARG  | NE-CZ-NH2  | -6.31 | 117.15      | 120.30   |
| 1   | B     | 483  | ARG  | NE-CZ-NH1  | -6.29 | 117.16      | 120.30   |
| 1   | B     | 86   | ALA  | CB-CA-C    | -6.27 | 100.70      | 110.10   |
| 1   | B     | 27   | ILE  | N-CA-CB    | -6.26 | 96.41       | 110.80   |
| 1   | B     | 1136 | VAL  | N-CA-CB    | 6.25  | 125.25      | 111.50   |
| 1   | B     | 1029 | VAL  | CA-CB-CG2  | 6.25  | 120.27      | 110.90   |
| 1   | A     | 822  | ARG  | NE-CZ-NH1  | -6.25 | 117.18      | 120.30   |
| 1   | B     | 479  | TYR  | CB-CG-CD1  | -6.25 | 117.25      | 121.00   |
| 1   | A     | 226  | PHE  | CB-CG-CD1  | -6.24 | 116.44      | 120.80   |
| 1   | B     | 919  | ASP  | CB-CG-OD1  | 6.24  | 123.91      | 118.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | B     | 392  | VAL  | N-CA-CB    | 6.22  | 125.19      | 111.50   |
| 1   | A     | 601  | MET  | C-N-CA     | -6.22 | 106.15      | 121.70   |
| 1   | A     | 558  | ARG  | NE-CZ-NH1  | -6.19 | 117.20      | 120.30   |
| 1   | A     | 823  | VAL  | CA-CB-CG2  | 6.13  | 120.09      | 110.90   |
| 1   | A     | 848  | ALA  | CA-C-O     | -6.12 | 107.25      | 120.10   |
| 1   | A     | 532  | ARG  | C-N-CA     | -6.12 | 106.40      | 121.70   |
| 1   | B     | 613  | LEU  | CA-CB-CG   | 6.12  | 129.37      | 115.30   |
| 1   | A     | 521  | ASP  | CB-CG-OD1  | 6.10  | 123.79      | 118.30   |
| 1   | B     | 465  | ILE  | CB-CA-C    | 6.09  | 123.78      | 111.60   |
| 1   | B     | 1124 | VAL  | CB-CA-C    | -6.09 | 99.83       | 111.40   |
| 1   | A     | 141  | LEU  | CA-CB-CG   | 6.08  | 129.27      | 115.30   |
| 1   | A     | 306  | ARG  | O-C-N      | 6.08  | 132.64      | 121.10   |
| 1   | B     | 456  | ASP  | CB-CG-OD2  | -6.07 | 112.84      | 118.30   |
| 1   | A     | 350  | GLU  | OE1-CD-OE2 | 6.07  | 130.58      | 123.30   |
| 1   | B     | 983  | ASP  | CB-CG-OD2  | 6.06  | 123.75      | 118.30   |
| 1   | B     | 486  | TYR  | CB-CG-CD2  | 6.04  | 124.62      | 121.00   |
| 1   | A     | 55   | THR  | OG1-CB-CG2 | -6.04 | 96.12       | 110.00   |
| 1   | B     | 1027 | ARG  | NE-CZ-NH1  | 6.02  | 123.31      | 120.30   |
| 1   | A     | 306  | ARG  | CA-C-O     | -6.00 | 107.51      | 120.10   |
| 1   | B     | 768  | ASP  | CB-CG-OD1  | -5.99 | 112.91      | 118.30   |
| 1   | B     | 1034 | TYR  | CB-CG-CD1  | -5.99 | 117.41      | 121.00   |
| 1   | A     | 456  | ASP  | CB-CA-C    | -5.98 | 98.44       | 110.40   |
| 1   | A     | 664  | ARG  | NH1-CZ-NH2 | 5.98  | 125.98      | 119.40   |
| 1   | B     | 229  | ARG  | NE-CZ-NH1  | 5.98  | 123.29      | 120.30   |
| 1   | B     | 967  | TYR  | CB-CG-CD2  | -5.97 | 117.42      | 121.00   |
| 1   | A     | 235  | TYR  | CB-CG-CD1  | -5.97 | 117.42      | 121.00   |
| 1   | A     | 1036 | TYR  | CB-CG-CD1  | -5.97 | 117.42      | 121.00   |
| 1   | B     | 264  | VAL  | N-CA-CB    | -5.96 | 98.39       | 111.50   |
| 1   | A     | 1077 | ARG  | CD-NE-CZ   | 5.95  | 131.93      | 123.60   |
| 1   | B     | 303  | ARG  | NE-CZ-NH1  | -5.95 | 117.33      | 120.30   |
| 1   | B     | 465  | ILE  | CA-CB-CG2  | 5.92  | 122.74      | 110.90   |
| 1   | B     | 636  | ASN  | CA-CB-CG   | -5.90 | 100.42      | 113.40   |
| 1   | A     | 456  | ASP  | CB-CG-OD2  | -5.89 | 113.00      | 118.30   |
| 1   | A     | 1027 | ARG  | CD-NE-CZ   | 5.89  | 131.84      | 123.60   |
| 1   | A     | 184  | GLU  | CA-CB-CG   | 5.86  | 126.30      | 113.40   |
| 1   | A     | 1077 | ARG  | NE-CZ-NH2  | -5.82 | 117.39      | 120.30   |
| 1   | B     | 1136 | VAL  | CG1-CB-CG2 | 5.82  | 120.21      | 110.90   |
| 1   | A     | 1149 | ARG  | NE-CZ-NH1  | 5.81  | 123.21      | 120.30   |
| 1   | B     | 82   | THR  | N-CA-CB    | 5.79  | 121.30      | 110.30   |
| 1   | A     | 303  | ARG  | NE-CZ-NH2  | 5.79  | 123.19      | 120.30   |
| 1   | A     | 754  | ILE  | CA-CB-CG2  | 5.78  | 122.46      | 110.90   |
| 1   | B     | 456  | ASP  | CB-CA-C    | -5.77 | 98.85       | 110.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | B     | 993  | VAL  | N-CA-CB    | -5.75 | 98.84       | 111.50   |
| 1   | B     | 138  | PHE  | CB-CG-CD2  | -5.73 | 116.79      | 120.80   |
| 1   | B     | 271  | ARG  | NE-CZ-NH1  | 5.73  | 123.16      | 120.30   |
| 1   | A     | 1216 | ARG  | NE-CZ-NH2  | 5.72  | 123.16      | 120.30   |
| 1   | B     | 608  | GLN  | CA-CB-CG   | 5.72  | 125.99      | 113.40   |
| 1   | A     | 204  | ARG  | NH1-CZ-NH2 | 5.71  | 125.69      | 119.40   |
| 1   | A     | 793  | ARG  | CG-CD-NE   | -5.71 | 99.81       | 111.80   |
| 1   | B     | 1149 | ARG  | NE-CZ-NH2  | -5.71 | 117.45      | 120.30   |
| 1   | A     | 154  | LEU  | CB-CG-CD2  | 5.69  | 120.68      | 111.00   |
| 1   | A     | 82   | THR  | N-CA-CB    | 5.68  | 121.10      | 110.30   |
| 1   | B     | 953  | THR  | CA-CB-OG1  | 5.67  | 120.90      | 109.00   |
| 1   | A     | 532  | ARG  | CA-C-N     | -5.65 | 104.77      | 117.20   |
| 1   | B     | 6    | MET  | CA-CB-CG   | 5.64  | 122.89      | 113.30   |
| 1   | B     | 180  | ILE  | CA-CB-CG2  | 5.63  | 122.16      | 110.90   |
| 1   | B     | 821  | VAL  | N-CA-CB    | 5.63  | 123.88      | 111.50   |
| 1   | A     | 48   | ARG  | CB-CG-CD   | -5.62 | 97.00       | 111.60   |
| 1   | B     | 910  | LEU  | CA-CB-CG   | 5.60  | 128.18      | 115.30   |
| 1   | A     | 31   | THR  | CA-C-O     | -5.58 | 108.37      | 120.10   |
| 1   | A     | 406  | ASP  | CB-CG-OD1  | -5.58 | 113.28      | 118.30   |
| 1   | A     | 27   | ILE  | N-CA-CB    | -5.58 | 97.98       | 110.80   |
| 1   | B     | 793  | ARG  | N-CA-CB    | -5.58 | 100.56      | 110.60   |
| 1   | B     | 392  | VAL  | CG1-CB-CG2 | 5.57  | 119.82      | 110.90   |
| 1   | A     | 831  | ARG  | NE-CZ-NH1  | -5.55 | 117.53      | 120.30   |
| 1   | A     | 986  | VAL  | CA-CB-CG1  | 5.53  | 119.19      | 110.90   |
| 1   | B     | 486  | TYR  | CB-CG-CD1  | -5.52 | 117.69      | 121.00   |
| 1   | A     | 351  | ARG  | CG-CD-NE   | 5.51  | 123.36      | 111.80   |
| 1   | B     | 1200 | THR  | CA-CB-CG2  | 5.49  | 120.08      | 112.40   |
| 1   | A     | 1221 | GLU  | CA-CB-CG   | 5.48  | 125.45      | 113.40   |
| 1   | A     | 1124 | VAL  | N-CA-CB    | 5.46  | 123.51      | 111.50   |
| 1   | A     | 960  | PHE  | CB-CG-CD1  | -5.45 | 116.99      | 120.80   |
| 1   | A     | 1147 | ARG  | CG-CD-NE   | -5.44 | 100.37      | 111.80   |
| 1   | A     | 175  | ARG  | NE-CZ-NH1  | -5.44 | 117.58      | 120.30   |
| 1   | B     | 479  | TYR  | CB-CG-CD2  | 5.42  | 124.25      | 121.00   |
| 1   | B     | 245  | GLU  | O-C-N      | -5.41 | 114.04      | 122.70   |
| 1   | A     | 264  | VAL  | N-CA-CB    | -5.41 | 99.60       | 111.50   |
| 1   | B     | 264  | VAL  | CB-CA-C    | 5.41  | 121.68      | 111.40   |
| 1   | A     | 329  | ARG  | CD-NE-CZ   | 5.40  | 131.16      | 123.60   |
| 1   | A     | 342  | LEU  | CB-CG-CD1  | 5.40  | 120.18      | 111.00   |
| 1   | B     | 1064 | LEU  | CA-CB-CG   | 5.39  | 127.70      | 115.30   |
| 1   | A     | 1108 | GLN  | CA-CB-CG   | 5.39  | 125.26      | 113.40   |
| 1   | B     | 754  | ILE  | CA-CB-CG2  | 5.39  | 121.67      | 110.90   |
| 1   | B     | 656  | VAL  | CA-CB-CG1  | 5.36  | 118.94      | 110.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 953  | THR  | CA-CB-OG1  | 5.35  | 120.23      | 109.00   |
| 1   | B     | 821  | VAL  | CA-CB-CG2  | 5.35  | 118.92      | 110.90   |
| 1   | A     | 356  | PRO  | CA-C-N     | 5.34  | 128.96      | 117.20   |
| 1   | A     | 637  | GLU  | N-CA-CB    | -5.33 | 101.00      | 110.60   |
| 1   | A     | 698  | VAL  | N-CA-CB    | -5.33 | 99.77       | 111.50   |
| 1   | B     | 960  | PHE  | CB-CG-CD1  | -5.33 | 117.07      | 120.80   |
| 1   | B     | 886  | ARG  | NE-CZ-NH1  | 5.32  | 122.96      | 120.30   |
| 1   | A     | 924  | LYS  | CD-CE-NZ   | 5.32  | 123.94      | 111.70   |
| 1   | A     | 637  | GLU  | CA-C-O     | -5.31 | 108.94      | 120.10   |
| 1   | A     | 1027 | ARG  | NE-CZ-NH2  | 5.31  | 122.95      | 120.30   |
| 1   | B     | 311  | GLU  | CA-CB-CG   | 5.31  | 125.08      | 113.40   |
| 1   | A     | 899  | GLU  | CA-CB-CG   | 5.30  | 125.06      | 113.40   |
| 1   | A     | 1187 | ASP  | CB-CG-OD2  | -5.27 | 113.56      | 118.30   |
| 1   | B     | 892  | ASP  | CB-CG-OD2  | 5.26  | 123.04      | 118.30   |
| 1   | A     | 919  | ASP  | OD1-CG-OD2 | -5.25 | 113.32      | 123.30   |
| 1   | B     | 307  | PRO  | N-CA-CB    | 5.25  | 109.61      | 103.30   |
| 1   | B     | 39   | GLU  | CA-CB-CG   | -5.25 | 101.85      | 113.40   |
| 1   | B     | 963  | ASP  | CB-CG-OD1  | 5.25  | 123.02      | 118.30   |
| 1   | A     | 967  | TYR  | CB-CG-CD1  | 5.25  | 124.15      | 121.00   |
| 1   | A     | 236  | TYR  | CD1-CG-CD2 | 5.24  | 123.66      | 117.90   |
| 1   | A     | 986  | VAL  | CA-CB-CG2  | 5.24  | 118.75      | 110.90   |
| 1   | A     | 479  | TYR  | CB-CG-CD2  | 5.24  | 124.14      | 121.00   |
| 1   | A     | 245  | GLU  | CA-CB-CG   | 5.23  | 124.92      | 113.40   |
| 1   | B     | 1047 | GLN  | CB-CG-CD   | 5.23  | 125.19      | 111.60   |
| 1   | A     | 456  | ASP  | CB-CG-OD1  | 5.22  | 122.99      | 118.30   |
| 1   | B     | 494  | TYR  | CB-CG-CD1  | -5.21 | 117.87      | 121.00   |
| 1   | B     | 134  | ARG  | CG-CD-NE   | 5.20  | 122.73      | 111.80   |
| 1   | B     | 712  | GLU  | C-N-CA     | -5.20 | 108.70      | 121.70   |
| 1   | B     | 581  | ASP  | CB-CG-OD1  | -5.20 | 113.62      | 118.30   |
| 1   | A     | 1136 | VAL  | N-CA-CB    | 5.19  | 122.92      | 111.50   |
| 1   | B     | 794  | ASP  | CB-CG-OD2  | 5.18  | 122.97      | 118.30   |
| 1   | B     | 1121 | ASP  | CB-CG-OD2  | 5.18  | 122.97      | 118.30   |
| 1   | B     | 223  | ASP  | CB-CG-OD1  | 5.18  | 122.96      | 118.30   |
| 1   | A     | 392  | VAL  | CA-CB-CG2  | 5.18  | 118.67      | 110.90   |
| 1   | B     | 329  | ARG  | NE-CZ-NH2  | -5.17 | 117.72      | 120.30   |
| 1   | A     | 1159 | ARG  | NE-CZ-NH2  | -5.17 | 117.72      | 120.30   |
| 1   | B     | 302  | VAL  | CA-CB-CG2  | 5.17  | 118.65      | 110.90   |
| 1   | B     | 673  | GLU  | OE1-CD-OE2 | -5.15 | 117.12      | 123.30   |
| 1   | B     | 1068 | TYR  | CB-CG-CD2  | 5.14  | 124.09      | 121.00   |
| 1   | A     | 399  | THR  | CA-CB-CG2  | -5.14 | 105.21      | 112.40   |
| 1   | A     | 952  | TYR  | CB-CG-CD1  | -5.13 | 117.92      | 121.00   |
| 1   | A     | 637  | GLU  | CB-CA-C    | -5.13 | 100.14      | 110.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | B     | 637  | GLU  | CG-CD-OE2  | -5.13 | 108.04      | 118.30   |
| 1   | B     | 14   | THR  | CA-CB-OG1  | 5.13  | 119.77      | 109.00   |
| 1   | B     | 1159 | ARG  | NE-CZ-NH2  | -5.12 | 117.74      | 120.30   |
| 1   | A     | 465  | ILE  | CA-CB-CG2  | 5.12  | 121.13      | 110.90   |
| 1   | A     | 229  | ARG  | NE-CZ-NH1  | 5.10  | 122.85      | 120.30   |
| 1   | B     | 1213 | ASP  | CB-CG-OD1  | 5.09  | 122.88      | 118.30   |
| 1   | A     | 236  | TYR  | CG-CD1-CE1 | -5.09 | 117.23      | 121.30   |
| 1   | A     | 1219 | THR  | OG1-CB-CG2 | 5.07  | 121.67      | 110.00   |
| 1   | A     | 465  | ILE  | CB-CA-C    | 5.05  | 121.71      | 111.60   |
| 1   | B     | 188  | TYR  | CB-CG-CD2  | -5.05 | 117.97      | 121.00   |
| 1   | B     | 211  | GLU  | CG-CD-OE2  | -5.04 | 108.22      | 118.30   |
| 1   | B     | 1124 | VAL  | CG1-CB-CG2 | 5.04  | 118.96      | 110.90   |
| 1   | A     | 1032 | TYR  | CG-CD2-CE2 | -5.03 | 117.27      | 121.30   |
| 1   | B     | 411  | ASP  | CB-CG-OD1  | 5.03  | 122.83      | 118.30   |
| 1   | A     | 8    | THR  | CB-CA-C    | -5.03 | 98.03       | 111.60   |
| 1   | B     | 1068 | TYR  | CB-CG-CD1  | -5.03 | 117.98      | 121.00   |
| 1   | B     | 911  | GLN  | CB-CG-CD   | 5.02  | 124.65      | 111.60   |
| 1   | B     | 302  | VAL  | CA-CB-CG1  | 5.01  | 118.42      | 110.90   |
| 1   | A     | 1199 | ASP  | CB-CG-OD2  | -5.01 | 113.79      | 118.30   |
| 1   | B     | 307  | PRO  | CA-N-CD    | -5.01 | 104.49      | 111.50   |
| 1   | B     | 637  | GLU  | CB-CG-CD   | 5.00  | 127.71      | 114.20   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | B     | 712 | GLU  | CA   |
| 1   | B     | 732 | LYS  | CA   |

All (5) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 532  | ARG  | Mainchain |
| 1   | A     | 637  | GLU  | Mainchain |
| 1   | B     | 1029 | VAL  | Mainchain |
| 1   | B     | 129  | ASP  | Mainchain |
| 1   | B     | 712  | GLU  | Mainchain |

## 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     | 9383  | 0        | 9263     | 237     | 0            |
| 1   | B     | 9383  | 0        | 9261     | 203     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 24    | 0        | 0        | 0       | 0            |
| 4   | B     | 24    | 0        | 0        | 0       | 0            |
| 5   | A     | 29    | 0        | 18       | 3       | 0            |
| 5   | B     | 29    | 0        | 18       | 2       | 0            |
| 6   | A     | 3     | 0        | 0        | 1       | 0            |
| 6   | B     | 3     | 0        | 0        | 1       | 0            |
| 7   | A     | 851   | 0        | 0        | 37      | 0            |
| 7   | B     | 1042  | 0        | 0        | 31      | 0            |
| All | All   | 20775 | 0        | 18560    | 414     | 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 11.

All (414) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:B:3236:HTL:C1'  | 5:B:3236:HTL:C2   | 1.94                     | 1.43              |
| 5:A:2236:HTL:C1'  | 5:A:2236:HTL:C2   | 1.97                     | 1.39              |
| 1:A:635:THR:HG22  | 1:A:640:LYS:HE2   | 1.34                     | 1.05              |
| 1:A:1219:THR:HG22 | 1:A:1222:GLN:H    | 1.23                     | 0.98              |
| 1:A:892:ASP:HB3   | 7:A:2415:HOH:O    | 1.70                     | 0.90              |
| 1:A:1132:ASN:HD21 | 1:A:1139:ARG:HH12 | 1.21                     | 0.89              |
| 1:A:398:VAL:HG13  | 1:A:656:VAL:HG22  | 1.54                     | 0.88              |
| 1:A:1181:LYS:H    | 1:B:1019:ARG:HH12 | 1.22                     | 0.87              |
| 1:A:883:MET:SD    | 7:B:3601:HOH:O    | 2.34                     | 0.86              |
| 1:B:874:GLU:HB3   | 7:B:4242:HOH:O    | 1.75                     | 0.86              |
| 1:A:883:MET:HE3   | 1:A:887:ARG:HD2   | 1.58                     | 0.83              |
| 1:A:1219:THR:HG21 | 7:B:3370:HOH:O    | 1.77                     | 0.83              |
| 1:B:1200:THR:HG23 | 1:B:1202:MET:H    | 1.42                     | 0.83              |
| 1:A:147:GLN:HE22  | 1:A:184:GLU:H     | 1.25                     | 0.82              |
| 1:B:883:MET:HE3   | 1:B:887:ARG:HD2   | 1.63                     | 0.81              |
| 1:A:841:SER:HB3   | 1:A:989:MET:HE1   | 1.61                     | 0.81              |
| 1:B:227:GLN:HE21  | 1:B:227:GLN:H     | 1.28                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:532:ARG:CA    | 1:A:533:THR:N     | 2.44                     | 0.80              |
| 1:A:227:GLN:H     | 1:A:227:GLN:HE21  | 1.29                     | 0.80              |
| 1:A:601:MET:CA    | 1:A:602:ASN:N     | 2.44                     | 0.80              |
| 1:B:1132:ASN:HD21 | 1:B:1139:ARG:HH12 | 1.28                     | 0.80              |
| 1:B:712:GLU:CA    | 1:B:713:GLU:N     | 2.45                     | 0.80              |
| 1:B:856:ASN:HD21  | 1:B:860:GLN:HE21  | 1.27                     | 0.80              |
| 1:B:147:GLN:HE22  | 1:B:184:GLU:H     | 1.32                     | 0.78              |
| 1:B:1189:GLY:HA3  | 1:B:1196:THR:HG21 | 1.66                     | 0.77              |
| 1:A:396:ASP:HA    | 1:A:656:VAL:HG13  | 1.65                     | 0.77              |
| 1:B:1173:GLU:HA   | 7:B:3899:HOH:O    | 1.86                     | 0.75              |
| 1:B:396:ASP:HA    | 1:B:656:VAL:HG13  | 1.67                     | 0.75              |
| 7:A:2814:HOH:O    | 1:B:883:MET:SD    | 2.45                     | 0.75              |
| 1:A:535:ALA:HB1   | 1:A:623:LYS:HG3   | 1.70                     | 0.74              |
| 1:A:765:GLN:HE22  | 1:B:1229:ARG:HH12 | 1.36                     | 0.73              |
| 1:B:712:GLU:CA    | 1:B:712:GLU:O     | 2.35                     | 0.73              |
| 1:B:110:HIS:HD2   | 1:B:169:HIS:HD2   | 1.37                     | 0.72              |
| 1:A:1107:ALA:HB2  | 1:A:1175:PHE:HB3  | 1.71                     | 0.72              |
| 1:A:1080:MET:H    | 1:B:1215:ASN:ND2  | 1.88                     | 0.72              |
| 1:B:608:GLN:HG3   | 7:B:4160:HOH:O    | 1.90                     | 0.72              |
| 1:A:198:LYS:H     | 1:A:198:LYS:HZ3   | 1.35                     | 0.72              |
| 1:B:202:GLU:HG2   | 7:B:4207:HOH:O    | 1.90                     | 0.71              |
| 1:A:601:MET:O     | 1:A:601:MET:CA    | 2.39                     | 0.71              |
| 1:A:643:VAL:HB    | 1:A:849:PRO:HB2   | 1.71                     | 0.70              |
| 1:A:856:ASN:HD21  | 1:A:860:GLN:HE21  | 1.39                     | 0.70              |
| 1:B:1189:GLY:CA   | 1:B:1196:THR:HG21 | 2.22                     | 0.70              |
| 1:A:325:THR:HG21  | 7:A:2328:HOH:O    | 1.92                     | 0.70              |
| 1:A:532:ARG:O     | 1:A:532:ARG:CA    | 2.40                     | 0.70              |
| 1:B:549:ILE:HG23  | 1:B:608:GLN:HG2   | 1.73                     | 0.69              |
| 1:B:198:LYS:H     | 1:B:198:LYS:HD2   | 1.57                     | 0.69              |
| 1:B:41:ASP:HA     | 1:B:58:ILE:HD12   | 1.73                     | 0.69              |
| 1:A:1200:THR:HG21 | 7:A:2647:HOH:O    | 1.92                     | 0.69              |
| 1:A:110:HIS:HD2   | 1:A:169:HIS:HD2   | 1.41                     | 0.69              |
| 1:B:1198:ASP:OD2  | 1:B:1200:THR:HB   | 1.92                     | 0.69              |
| 1:A:1028:MET:HE2  | 1:B:1028:MET:HE2  | 1.73                     | 0.69              |
| 1:B:691:GLN:HE22  | 1:B:726:ALA:HA    | 1.57                     | 0.68              |
| 7:A:2929:HOH:O    | 1:B:1180:GLY:HA3  | 1.94                     | 0.68              |
| 1:A:1215:ASN:ND2  | 1:B:1080:MET:H    | 1.91                     | 0.68              |
| 1:B:986:VAL:HG22  | 1:B:1064:LEU:HD23 | 1.75                     | 0.67              |
| 1:A:1219:THR:HG22 | 1:A:1222:GLN:N    | 2.05                     | 0.67              |
| 1:A:765:GLN:NE2   | 1:B:1229:ARG:HH12 | 1.92                     | 0.67              |
| 1:B:636:ASN:HB3   | 1:B:639:PHE:H     | 1.60                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:463:ILE:HD11  | 1:A:465:ILE:HG22  | 1.76                     | 0.67              |
| 1:A:883:MET:CE    | 1:A:887:ARG:HD2   | 2.25                     | 0.67              |
| 1:A:1200:THR:HG23 | 1:A:1202:MET:H    | 1.60                     | 0.67              |
| 1:A:1198:ASP:OD2  | 1:A:1200:THR:HB   | 1.94                     | 0.67              |
| 1:A:1077:ARG:HH11 | 1:A:1077:ARG:HB2  | 1.58                     | 0.66              |
| 1:B:509:THR:HG21  | 7:B:3646:HOH:O    | 1.95                     | 0.66              |
| 1:A:509:THR:HG21  | 7:A:2978:HOH:O    | 1.96                     | 0.66              |
| 1:A:55:THR:HG22   | 7:A:2794:HOH:O    | 1.94                     | 0.66              |
| 1:B:325:THR:HG21  | 7:B:3257:HOH:O    | 1.95                     | 0.66              |
| 1:A:1132:ASN:O    | 1:A:1136:VAL:HG22 | 1.97                     | 0.65              |
| 1:A:606:VAL:O     | 1:A:610:VAL:HG23  | 1.97                     | 0.65              |
| 1:A:986:VAL:HG22  | 1:A:1064:LEU:HD23 | 1.78                     | 0.65              |
| 1:A:445:THR:HG21  | 1:A:574:LEU:HD21  | 1.77                     | 0.64              |
| 1:A:1102:ASP:OD1  | 1:A:1104:ARG:HG2  | 1.96                     | 0.64              |
| 1:A:444:ASN:HB2   | 1:A:582:LEU:HD21  | 1.80                     | 0.63              |
| 1:B:7:THR:HB      | 1:B:180:ILE:HD11  | 1.79                     | 0.62              |
| 1:B:883:MET:CE    | 1:B:887:ARG:HD2   | 2.29                     | 0.62              |
| 1:B:10:GLY:O      | 1:B:14:THR:HG23   | 2.00                     | 0.62              |
| 1:B:891:ALA:HB2   | 1:B:917:LYS:HZ1   | 1.64                     | 0.62              |
| 1:A:8:THR:HG22    | 7:A:2981:HOH:O    | 1.99                     | 0.62              |
| 1:A:14:THR:HG21   | 1:A:171:PHE:CE2   | 2.35                     | 0.62              |
| 1:A:691:GLN:HE22  | 1:A:726:ALA:HA    | 1.65                     | 0.61              |
| 1:B:643:VAL:HB    | 1:B:849:PRO:HB2   | 1.80                     | 0.61              |
| 1:A:1162:GLU:HG2  | 7:B:4112:HOH:O    | 1.98                     | 0.61              |
| 1:A:1189:GLY:CA   | 1:A:1196:THR:HG21 | 2.29                     | 0.61              |
| 1:A:635:THR:HG23  | 1:A:639:PHE:HB3   | 1.83                     | 0.61              |
| 1:B:780:TYR:HA    | 1:B:783:ARG:HH11  | 1.66                     | 0.60              |
| 1:B:5:MET:CE      | 1:B:184:GLU:HB2   | 2.32                     | 0.60              |
| 1:A:416:GLY:C     | 7:A:3044:HOH:O    | 2.39                     | 0.60              |
| 1:A:1080:MET:H    | 1:B:1215:ASN:HD21 | 1.51                     | 0.59              |
| 1:A:110:HIS:HD2   | 1:A:169:HIS:CD2   | 2.17                     | 0.59              |
| 1:A:14:THR:HG22   | 1:A:149:ALA:HB1   | 1.83                     | 0.59              |
| 1:B:9:ASP:OD2     | 1:B:12:THR:HG23   | 2.01                     | 0.59              |
| 1:B:311:GLU:HB3   | 7:B:4077:HOH:O    | 2.00                     | 0.59              |
| 1:A:639:PHE:HA    | 1:A:643:VAL:HG13  | 1.84                     | 0.59              |
| 1:B:398:VAL:HG13  | 1:B:656:VAL:HG22  | 1.84                     | 0.59              |
| 1:A:691:GLN:HE22  | 1:A:727:LYS:H     | 1.51                     | 0.59              |
| 1:B:110:HIS:HE1   | 1:B:157:HIS:NE2   | 2.01                     | 0.58              |
| 1:A:1054:LYS:HB2  | 7:A:2568:HOH:O    | 2.02                     | 0.58              |
| 1:A:351:ARG:HD2   | 7:A:2281:HOH:O    | 2.03                     | 0.58              |
| 1:A:1003:LYS:NZ   | 1:B:976:HIS:HD2   | 2.02                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:883:MET:HE1  | 1:B:955:LYS:HG3   | 1.86                     | 0.58              |
| 1:B:5:MET:HE1    | 1:B:184:GLU:HB2   | 1.84                     | 0.58              |
| 1:B:1187:ASP:HB3 | 1:B:1190:GLU:HG3  | 1.85                     | 0.57              |
| 7:A:2421:HOH:O   | 1:B:953:THR:HG21  | 2.04                     | 0.57              |
| 1:A:642:VAL:C    | 1:A:645:PRO:HD2   | 2.25                     | 0.57              |
| 1:B:1102:ASP:OD1 | 1:B:1104:ARG:HG2  | 2.04                     | 0.57              |
| 1:A:273:ILE:HG23 | 1:A:327:LEU:HD22  | 1.87                     | 0.57              |
| 1:A:325:THR:HG23 | 1:A:382:MET:SD    | 2.45                     | 0.57              |
| 1:B:43:TRP:HB3   | 1:B:48:ARG:HD2    | 1.87                     | 0.57              |
| 1:A:16:HIS:HD2   | 7:A:2251:HOH:O    | 1.87                     | 0.57              |
| 1:A:691:GLN:NE2  | 1:A:727:LYS:H     | 2.02                     | 0.56              |
| 1:A:644:LYS:N    | 1:A:645:PRO:CD    | 2.68                     | 0.56              |
| 1:B:737:ARG:HE   | 1:B:739:GLN:NE2   | 2.02                     | 0.56              |
| 1:A:1189:GLY:HA3 | 1:A:1196:THR:HG21 | 1.87                     | 0.56              |
| 1:A:953:THR:HG21 | 7:B:3491:HOH:O    | 2.06                     | 0.56              |
| 1:B:467:HIS:CD2  | 1:B:481:VAL:H     | 2.24                     | 0.56              |
| 1:A:398:VAL:CG1  | 1:A:656:VAL:HG22  | 2.32                     | 0.56              |
| 1:A:227:GLN:H    | 1:A:227:GLN:NE2   | 2.00                     | 0.55              |
| 1:A:686:PRO:HB2  | 1:A:724:LEU:HD21  | 1.87                     | 0.55              |
| 1:B:871:ASP:O    | 1:B:874:GLU:HG2   | 2.06                     | 0.55              |
| 1:B:780:TYR:HA   | 1:B:783:ARG:HD2   | 1.87                     | 0.55              |
| 1:A:1123:SER:O   | 1:A:1126:GLU:HG2  | 2.06                     | 0.55              |
| 1:B:821:VAL:HG12 | 1:B:989:MET:HE3   | 1.88                     | 0.55              |
| 1:B:16:HIS:HD2   | 7:B:3275:HOH:O    | 1.87                     | 0.55              |
| 1:A:212:HIS:HE1  | 1:B:950:ASP:OD2   | 1.87                     | 0.55              |
| 1:B:456:ASP:OD1  | 1:B:463:ILE:HG22  | 2.06                     | 0.55              |
| 1:A:1015:ALA:HB1 | 1:B:1185:SER:HB2  | 1.88                     | 0.55              |
| 1:A:10:GLY:O     | 1:A:14:THR:HG23   | 2.06                     | 0.55              |
| 1:A:467:HIS:CD2  | 1:A:481:VAL:H     | 2.25                     | 0.55              |
| 1:A:418:ILE:HD12 | 1:A:418:ILE:N     | 2.22                     | 0.54              |
| 1:A:1166:MET:O   | 1:A:1169:THR:HG22 | 2.06                     | 0.54              |
| 1:A:950:ASP:OD2  | 1:B:212:HIS:HE1   | 1.89                     | 0.54              |
| 1:B:14:THR:HG21  | 1:B:171:PHE:CE2   | 2.43                     | 0.54              |
| 1:B:1132:ASN:O   | 1:B:1136:VAL:HG22 | 2.08                     | 0.54              |
| 1:B:91:LEU:HD11  | 1:B:116:ILE:HD12  | 1.90                     | 0.54              |
| 1:B:14:THR:HG22  | 1:B:149:ALA:HB1   | 1.89                     | 0.54              |
| 1:A:1181:LYS:H   | 1:B:1019:ARG:NH1  | 1.99                     | 0.54              |
| 1:A:9:ASP:OD2    | 1:A:12:THR:HG23   | 2.07                     | 0.54              |
| 1:A:775:VAL:N    | 1:A:776:PRO:HD2   | 2.23                     | 0.54              |
| 1:A:411:ASP:HB2  | 1:A:483:ARG:HD2   | 1.89                     | 0.54              |
| 1:A:821:VAL:HG21 | 1:A:844:TRP:CH2   | 2.43                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:635:THR:HG23  | 1:A:636:ASN:H     | 1.73                     | 0.53              |
| 1:A:135:GLN:NE2   | 1:A:135:GLN:H     | 2.06                     | 0.53              |
| 1:B:212:HIS:HD2   | 7:B:3461:HOH:O    | 1.91                     | 0.53              |
| 1:A:7:THR:HB      | 1:A:180:ILE:HD11  | 1.90                     | 0.53              |
| 1:A:110:HIS:HE1   | 1:A:157:HIS:NE2   | 2.06                     | 0.53              |
| 1:A:737:ARG:HE    | 1:A:739:GLN:NE2   | 2.06                     | 0.53              |
| 1:A:927:GLY:O     | 1:A:931:LYS:HG3   | 2.08                     | 0.53              |
| 1:B:805:LEU:HB2   | 1:B:825:THR:HB    | 1.91                     | 0.53              |
| 1:A:1111:ASN:HD21 | 1:A:1169:THR:HG23 | 1.74                     | 0.52              |
| 1:B:544:ILE:HD12  | 1:B:613:LEU:HD13  | 1.91                     | 0.52              |
| 1:A:697:PHE:CD2   | 1:A:1046:LYS:HD3  | 2.44                     | 0.52              |
| 1:B:775:VAL:HB    | 1:B:776:PRO:HD3   | 1.91                     | 0.52              |
| 1:A:444:ASN:CB    | 1:A:582:LEU:HD21  | 2.39                     | 0.52              |
| 1:A:124:PHE:HB3   | 1:A:367:SER:HB2   | 1.91                     | 0.52              |
| 1:B:509:THR:HG22  | 7:B:3921:HOH:O    | 2.09                     | 0.52              |
| 1:B:780:TYR:CA    | 1:B:783:ARG:HH11  | 2.22                     | 0.52              |
| 1:B:1200:THR:CG2  | 1:B:1202:MET:H    | 2.20                     | 0.52              |
| 1:B:639:PHE:HA    | 1:B:643:VAL:HG13  | 1.90                     | 0.52              |
| 1:B:1035:VAL:HG22 | 1:B:1062:PRO:HG2  | 1.92                     | 0.52              |
| 1:B:691:GLN:NE2   | 1:B:727:LYS:H     | 2.07                     | 0.52              |
| 1:B:698:VAL:HG22  | 1:B:1084:GLN:CD   | 2.30                     | 0.52              |
| 1:B:779:GLU:C     | 1:B:783:ARG:HH11  | 2.13                     | 0.52              |
| 1:A:561:MET:HE1   | 1:A:583:LEU:HD22  | 1.92                     | 0.52              |
| 1:B:351:ARG:HD2   | 7:B:3509:HOH:O    | 2.10                     | 0.51              |
| 1:A:937:GLN:HG2   | 1:A:942:LEU:HB3   | 1.91                     | 0.51              |
| 1:A:1189:GLY:HA2  | 1:A:1196:THR:HG21 | 1.90                     | 0.51              |
| 1:A:456:ASP:HB2   | 7:B:3660:HOH:O    | 2.10                     | 0.51              |
| 1:B:351:ARG:HD3   | 1:B:353:GLU:HB2   | 1.92                     | 0.51              |
| 1:B:135:GLN:NE2   | 1:B:135:GLN:H     | 2.09                     | 0.51              |
| 1:B:390:PHE:CD1   | 1:B:403:LEU:HD22  | 2.46                     | 0.51              |
| 1:A:1129:MET:CE   | 1:A:1149:ARG:HD3  | 2.41                     | 0.51              |
| 1:B:989:MET:SD    | 7:B:3942:HOH:O    | 2.59                     | 0.51              |
| 1:A:212:HIS:HD2   | 7:A:2694:HOH:O    | 1.94                     | 0.51              |
| 1:B:1077:ARG:HH11 | 1:B:1077:ARG:HB2  | 1.76                     | 0.51              |
| 1:B:691:GLN:HE22  | 1:B:727:LYS:H     | 1.59                     | 0.51              |
| 1:B:536:ASN:HD22  | 1:B:623:LYS:NZ    | 2.09                     | 0.51              |
| 1:A:636:ASN:HB3   | 1:A:638:PHE:H     | 1.76                     | 0.50              |
| 1:A:1111:ASN:ND2  | 1:A:1169:THR:HG23 | 2.26                     | 0.50              |
| 1:A:953:THR:HG22  | 7:A:2274:HOH:O    | 2.11                     | 0.50              |
| 1:B:1029:VAL:HG22 | 1:B:1037:VAL:CG2  | 2.41                     | 0.50              |
| 1:A:989:MET:HE2   | 7:A:3079:HOH:O    | 2.12                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:110:HIS:HD2   | 1:B:169:HIS:CD2   | 2.24                     | 0.50              |
| 1:A:630:LYS:C     | 1:A:632:GLU:H     | 2.14                     | 0.50              |
| 1:A:918:ASN:O     | 1:A:954:LYS:HD2   | 2.12                     | 0.50              |
| 1:A:7:THR:OG1     | 1:A:439:LYS:HE3   | 2.11                     | 0.50              |
| 1:A:1129:MET:HE2  | 1:A:1149:ARG:HD3  | 1.94                     | 0.50              |
| 1:B:637:GLU:HG2   | 1:B:638:PHE:N     | 2.27                     | 0.50              |
| 1:B:1029:VAL:HG22 | 1:B:1037:VAL:HG22 | 1.93                     | 0.49              |
| 1:B:233:ASN:HB2   | 1:B:234:PRO:HD3   | 1.92                     | 0.49              |
| 1:B:636:ASN:HB2   | 1:B:639:PHE:HB2   | 1.93                     | 0.49              |
| 1:B:322:LYS:O     | 1:B:356:PRO:O     | 2.29                     | 0.49              |
| 1:A:1129:MET:HE1  | 1:A:1135:ALA:HA   | 1.95                     | 0.49              |
| 1:A:756:PRO:N     | 1:A:757:PRO:HD2   | 2.27                     | 0.49              |
| 1:B:1000:GLN:HG3  | 1:B:1012:LYS:HB2  | 1.94                     | 0.49              |
| 1:B:554:GLY:HA3   | 1:B:601:MET:HE2   | 1.94                     | 0.49              |
| 7:A:2819:HOH:O    | 1:B:1221:GLU:HG2  | 2.12                     | 0.49              |
| 1:B:883:MET:CE    | 1:B:955:LYS:HG3   | 2.42                     | 0.49              |
| 1:A:467:HIS:HD2   | 1:A:481:VAL:H     | 1.59                     | 0.49              |
| 1:A:227:GLN:HE21  | 1:A:227:GLN:N     | 2.05                     | 0.49              |
| 1:A:16:HIS:HE1    | 1:A:186:LEU:O     | 1.96                     | 0.49              |
| 1:A:110:HIS:CD2   | 1:A:169:HIS:HD2   | 2.26                     | 0.49              |
| 1:A:463:ILE:CD1   | 1:A:465:ILE:HG22  | 2.43                     | 0.49              |
| 1:B:718:PRO:HG2   | 1:B:777:ASN:HD22  | 1.77                     | 0.49              |
| 1:A:135:GLN:HG2   | 7:A:2668:HOH:O    | 2.12                     | 0.49              |
| 1:A:1202:MET:HG2  | 6:B:3240:CO2:O2   | 2.13                     | 0.48              |
| 1:A:773:ALA:O     | 1:A:776:PRO:HD2   | 2.13                     | 0.48              |
| 1:B:431:VAL:CG2   | 1:B:464:THR:HG21  | 2.43                     | 0.48              |
| 1:A:818:THR:HA    | 1:A:821:VAL:HG22  | 1.95                     | 0.48              |
| 1:A:221:ASN:HB3   | 1:A:222:PRO:CD    | 2.43                     | 0.48              |
| 1:B:467:HIS:HD2   | 1:B:481:VAL:H     | 1.59                     | 0.48              |
| 1:A:1111:ASN:HD21 | 1:A:1169:THR:CG2  | 2.26                     | 0.48              |
| 1:B:1146:LYS:HD3  | 7:B:3988:HOH:O    | 2.12                     | 0.48              |
| 1:A:389:HIS:HD2   | 7:A:2627:HOH:O    | 1.97                     | 0.48              |
| 1:A:869:PHE:CE2   | 1:A:969:ILE:HG21  | 2.48                     | 0.48              |
| 1:A:780:TYR:HA    | 1:A:783:ARG:HD2   | 1.95                     | 0.48              |
| 1:B:639:PHE:CE1   | 1:B:643:VAL:HG22  | 2.48                     | 0.48              |
| 1:A:351:ARG:NH1   | 1:A:354:ALA:O     | 2.47                     | 0.48              |
| 1:A:1154:HIS:HE1  | 1:B:1174:SER:HB2  | 1.78                     | 0.48              |
| 7:A:2373:HOH:O    | 1:B:1028:MET:HE3  | 2.14                     | 0.48              |
| 1:A:569:LYS:NZ    | 1:A:610:VAL:O     | 2.47                     | 0.48              |
| 1:A:8:THR:HG21    | 1:A:12:THR:OG1    | 2.14                     | 0.48              |
| 1:A:1219:THR:CG2  | 1:A:1221:GLU:HG2  | 2.44                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:473:LYS:HB3   | 1:A:474:PRO:HD2   | 1.96                     | 0.48              |
| 1:B:3:LYS:HB3     | 1:B:184:GLU:HG3   | 1.95                     | 0.47              |
| 1:B:110:HIS:CD2   | 1:B:169:HIS:HD2   | 2.26                     | 0.47              |
| 1:B:953:THR:HG22  | 7:B:3279:HOH:O    | 2.14                     | 0.47              |
| 1:B:1129:MET:CE   | 1:B:1149:ARG:HD3  | 2.44                     | 0.47              |
| 1:A:909:ALA:CB    | 1:A:930:LEU:HD13  | 2.44                     | 0.47              |
| 1:B:594:LYS:N     | 7:B:3668:HOH:O    | 2.47                     | 0.47              |
| 1:A:331:LYS:HD3   | 1:A:362:ARG:CZ    | 2.45                     | 0.47              |
| 1:A:1185:SER:HB3  | 1:B:45:ALA:HB3    | 1.95                     | 0.47              |
| 7:A:2345:HOH:O    | 1:B:229:ARG:HD2   | 2.15                     | 0.47              |
| 1:A:821:VAL:HG21  | 1:A:844:TRP:HH2   | 1.79                     | 0.47              |
| 1:B:198:LYS:HD2   | 1:B:198:LYS:N     | 2.28                     | 0.47              |
| 1:A:27:ILE:HG13   | 7:A:2418:HOH:O    | 2.13                     | 0.47              |
| 1:A:805:LEU:HB2   | 1:A:825:THR:HB    | 1.96                     | 0.47              |
| 1:A:507:GLY:HA2   | 1:A:538:LYS:O     | 2.15                     | 0.47              |
| 1:B:1040:VAL:HG12 | 1:B:1048:GLN:HE22 | 1.80                     | 0.47              |
| 1:A:273:ILE:CG2   | 1:A:327:LEU:HD22  | 2.45                     | 0.47              |
| 1:B:910:LEU:HD13  | 1:B:930:LEU:HD11  | 1.96                     | 0.46              |
| 1:A:390:PHE:CD1   | 1:A:403:LEU:HD22  | 2.49                     | 0.46              |
| 1:A:90:LEU:HD11   | 1:A:168:MET:CE    | 2.46                     | 0.46              |
| 1:A:1003:LYS:HZ3  | 1:B:976:HIS:HD2   | 1.63                     | 0.46              |
| 1:B:1042:MET:HG2  | 1:B:1084:GLN:HE22 | 1.80                     | 0.46              |
| 1:A:390:PHE:CE1   | 1:A:403:LEU:HD22  | 2.51                     | 0.46              |
| 1:A:1186:VAL:HG23 | 1:A:1190:GLU:OE1  | 2.15                     | 0.46              |
| 1:A:561:MET:HE1   | 1:A:583:LEU:CD2   | 2.45                     | 0.46              |
| 1:B:554:GLY:HA3   | 1:B:601:MET:CE    | 2.46                     | 0.46              |
| 1:A:240:PRO:HB3   | 1:A:309:VAL:HG21  | 1.97                     | 0.46              |
| 1:A:350:GLU:CD    | 1:B:389:HIS:HE1   | 2.19                     | 0.46              |
| 1:A:12:THR:HB     | 1:A:39:GLU:OE2    | 2.15                     | 0.46              |
| 1:A:465:ILE:HG13  | 1:A:467:HIS:CE1   | 2.51                     | 0.46              |
| 1:A:9:ASP:HA      | 1:A:179:GLU:O     | 2.15                     | 0.46              |
| 1:A:739:GLN:NE2   | 1:A:777:ASN:HB3   | 2.31                     | 0.46              |
| 1:A:342:LEU:HD12  | 1:B:346:SER:HB3   | 1.97                     | 0.46              |
| 1:B:802:GLN:NE2   | 7:B:4051:HOH:O    | 2.43                     | 0.46              |
| 1:A:841:SER:HA    | 1:A:844:TRP:CE2   | 2.51                     | 0.46              |
| 1:A:775:VAL:N     | 1:A:776:PRO:CD    | 2.79                     | 0.46              |
| 1:A:5:MET:HE1     | 7:A:3054:HOH:O    | 2.15                     | 0.46              |
| 1:B:891:ALA:CB    | 1:B:917:LYS:HZ1   | 2.29                     | 0.46              |
| 1:B:544:ILE:CD1   | 1:B:613:LEU:HD13  | 2.46                     | 0.46              |
| 1:A:198:LYS:N     | 1:A:198:LYS:HZ3   | 2.09                     | 0.46              |
| 1:B:1197:ARG:HD3  | 7:B:4066:HOH:O    | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:732:LYS:CA    | 1:B:732:LYS:CD    | 2.93                     | 0.46              |
| 1:A:325:THR:CG2   | 1:A:382:MET:SD    | 3.04                     | 0.45              |
| 1:A:108:VAL:HG21  | 1:A:157:HIS:HA    | 1.98                     | 0.45              |
| 1:A:1077:ARG:HD2  | 7:A:3041:HOH:O    | 2.16                     | 0.45              |
| 1:A:729:LYS:O     | 1:A:732:LYS:HE2   | 2.16                     | 0.45              |
| 1:A:976:HIS:HD2   | 1:B:1003:LYS:NZ   | 2.13                     | 0.45              |
| 1:A:421:GLN:NE2   | 7:A:2725:HOH:O    | 2.50                     | 0.45              |
| 1:A:355:MET:HA    | 1:A:356:PRO:HD2   | 1.86                     | 0.45              |
| 1:A:588:HIS:CD2   | 1:A:599:VAL:HG11  | 2.51                     | 0.45              |
| 1:A:639:PHE:CE1   | 1:A:672:PHE:HB2   | 2.51                     | 0.45              |
| 1:B:227:GLN:NE2   | 1:B:227:GLN:H     | 2.05                     | 0.45              |
| 1:A:775:VAL:O     | 1:A:779:GLU:HG2   | 2.16                     | 0.45              |
| 1:B:841:SER:HA    | 1:B:844:TRP:CE2   | 2.51                     | 0.45              |
| 1:B:1104:ARG:HB2  | 7:B:4216:HOH:O    | 2.16                     | 0.45              |
| 1:B:780:TYR:N     | 1:B:783:ARG:HH11  | 2.14                     | 0.45              |
| 1:B:423:TRP:CE3   | 1:B:463:ILE:HD11  | 2.52                     | 0.45              |
| 1:A:1231:LYS:O    | 1:A:1232:LYS:HB2  | 2.17                     | 0.45              |
| 1:A:818:THR:OG1   | 1:A:819:PRO:HD3   | 2.17                     | 0.45              |
| 1:B:1104:ARG:O    | 1:B:1108:GLN:HG3  | 2.17                     | 0.45              |
| 1:B:465:ILE:HG13  | 1:B:467:HIS:CE1   | 2.52                     | 0.45              |
| 1:A:221:ASN:HB3   | 1:A:222:PRO:HD2   | 2.00                     | 0.44              |
| 1:B:1129:MET:HE1  | 1:B:1149:ARG:HD3  | 1.98                     | 0.44              |
| 1:B:389:HIS:HD2   | 7:B:3639:HOH:O    | 2.00                     | 0.44              |
| 1:A:431:VAL:CG2   | 1:A:464:THR:HG21  | 2.47                     | 0.44              |
| 1:A:497:ILE:HG13  | 1:A:498:TYR:CD1   | 2.53                     | 0.44              |
| 1:A:1078:LYS:O    | 1:B:1219:THR:HG23 | 2.18                     | 0.44              |
| 1:A:266:ALA:HA    | 1:A:267:PRO:HD3   | 1.83                     | 0.44              |
| 1:A:560:ASN:H     | 1:A:560:ASN:HD22  | 1.65                     | 0.44              |
| 1:B:578:LYS:HG2   | 1:B:582:LEU:HD22  | 1.98                     | 0.44              |
| 1:A:1196:THR:HG22 | 7:A:2483:HOH:O    | 2.16                     | 0.44              |
| 1:A:357:LYS:HE3   | 1:A:359:LEU:HD13  | 1.98                     | 0.44              |
| 1:B:1177:PRO:O    | 1:B:1178:ALA:HB2  | 2.17                     | 0.44              |
| 1:A:389:HIS:HE1   | 1:B:350:GLU:CD    | 2.21                     | 0.44              |
| 1:B:495:VAL:HG13  | 1:B:527:PRO:HD3   | 2.00                     | 0.44              |
| 1:A:1219:THR:CG2  | 1:A:1222:GLN:H    | 2.11                     | 0.44              |
| 1:A:1180:GLY:H    | 1:A:1181:LYS:HZ1  | 1.65                     | 0.44              |
| 1:A:1143:GLU:HG2  | 7:A:3066:HOH:O    | 2.18                     | 0.44              |
| 1:A:465:ILE:HG12  | 7:A:2473:HOH:O    | 2.17                     | 0.44              |
| 1:B:536:ASN:HA    | 1:B:623:LYS:HZ3   | 1.83                     | 0.43              |
| 1:A:576:PHE:O     | 1:A:580:VAL:HG23  | 2.18                     | 0.43              |
| 1:A:635:THR:HG23  | 1:A:636:ASN:N     | 2.33                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:871:ASP:HB2   | 1:B:874:GLU:HG2   | 1.99                     | 0.43              |
| 1:A:82:THR:HG22   | 1:A:108:VAL:O     | 2.18                     | 0.43              |
| 1:A:650:GLN:OE1   | 1:A:653:LYS:HE3   | 2.19                     | 0.43              |
| 1:A:1199:ASP:CG   | 1:A:1214:GLN:HE22 | 2.21                     | 0.43              |
| 1:B:27:ILE:HD11   | 1:B:84:PHE:CD1    | 2.54                     | 0.43              |
| 1:B:779:GLU:C     | 1:B:783:ARG:NH1   | 2.72                     | 0.43              |
| 1:B:739:GLN:NE2   | 1:B:777:ASN:HB3   | 2.34                     | 0.43              |
| 1:B:821:VAL:CG1   | 1:B:989:MET:CE    | 2.96                     | 0.43              |
| 1:B:906:VAL:HG12  | 1:B:910:LEU:HD22  | 2.00                     | 0.43              |
| 1:A:487:VAL:O     | 1:A:510:PHE:HA    | 2.19                     | 0.43              |
| 1:A:1219:THR:HG23 | 1:A:1221:GLU:HG2  | 2.00                     | 0.43              |
| 1:B:644:LYS:N     | 1:B:645:PRO:CD    | 2.82                     | 0.43              |
| 1:B:491:ASN:HD22  | 1:B:492:PRO:HD2   | 1.82                     | 0.43              |
| 1:A:180:ILE:HD12  | 1:A:181:GLN:N     | 2.34                     | 0.43              |
| 1:B:775:VAL:N     | 1:B:776:PRO:CD    | 2.82                     | 0.43              |
| 1:A:639:PHE:CE1   | 1:A:643:VAL:HG22  | 2.53                     | 0.43              |
| 1:B:1200:THR:HG22 | 1:B:1203:MET:H    | 1.83                     | 0.43              |
| 1:A:1215:ASN:HD21 | 1:B:1079:GLY:HA2  | 1.84                     | 0.43              |
| 1:A:574:LEU:HD13  | 1:A:578:LYS:HG2   | 2.01                     | 0.43              |
| 1:A:590:ALA:O     | 1:A:591:TYR:HB2   | 2.18                     | 0.43              |
| 1:A:601:MET:N     | 1:A:602:ASN:N     | 2.67                     | 0.42              |
| 1:B:779:GLU:O     | 1:B:783:ARG:HD2   | 2.19                     | 0.42              |
| 1:B:1219:THR:O    | 1:B:1223:GLN:HG3  | 2.19                     | 0.42              |
| 1:A:357:LYS:HD2   | 7:A:2763:HOH:O    | 2.18                     | 0.42              |
| 1:A:534:ILE:HA    | 1:A:539:LEU:HD12  | 2.01                     | 0.42              |
| 1:A:331:LYS:HD2   | 7:A:2573:HOH:O    | 2.19                     | 0.42              |
| 1:A:1200:THR:CG2  | 1:A:1202:MET:HB2  | 2.50                     | 0.42              |
| 1:B:821:VAL:CG1   | 1:B:989:MET:HE3   | 2.49                     | 0.42              |
| 1:A:1229:ARG:HH12 | 1:B:765:GLN:HE22  | 1.67                     | 0.42              |
| 1:A:1200:THR:HG23 | 1:A:1202:MET:HE3  | 2.01                     | 0.42              |
| 1:B:1165:HIS:O    | 1:B:1165:HIS:CG   | 2.72                     | 0.42              |
| 1:A:1028:MET:CE   | 1:B:1028:MET:HB3  | 2.49                     | 0.42              |
| 1:A:61:MET:HG3    | 1:A:67:ALA:HA     | 2.01                     | 0.42              |
| 1:B:141:LEU:HD13  | 1:B:152:MET:HB3   | 2.01                     | 0.42              |
| 1:B:37:GLY:HA3    | 7:B:4020:HOH:O    | 2.20                     | 0.42              |
| 1:A:841:SER:HB3   | 1:A:989:MET:CE    | 2.42                     | 0.42              |
| 1:A:61:MET:HA     | 1:B:976:HIS:CE1   | 2.54                     | 0.42              |
| 1:B:574:LEU:HB3   | 1:B:575:PRO:HD2   | 2.02                     | 0.42              |
| 1:A:12:THR:CG2    | 1:A:39:GLU:OE2    | 2.68                     | 0.42              |
| 1:A:1015:ALA:CB   | 1:B:1185:SER:HB2  | 2.50                     | 0.42              |
| 1:B:699:CYS:HA    | 1:B:700:PRO:HD3   | 1.80                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:562:ILE:HD12  | 1:A:562:ILE:N     | 2.35                     | 0.42              |
| 1:A:681:VAL:HB    | 1:A:682:PRO:HD2   | 2.00                     | 0.42              |
| 1:B:779:GLU:HB3   | 1:B:783:ARG:NH1   | 2.35                     | 0.42              |
| 1:B:536:ASN:HD22  | 1:B:623:LYS:HZ3   | 1.66                     | 0.42              |
| 1:B:601:MET:HE1   | 7:B:3967:HOH:O    | 2.19                     | 0.42              |
| 1:A:650:GLN:CD    | 1:A:653:LYS:HE3   | 2.39                     | 0.42              |
| 1:A:754:ILE:HD13  | 1:A:1084:GLN:HB2  | 2.02                     | 0.42              |
| 1:B:1166:MET:O    | 1:B:1169:THR:HG22 | 2.20                     | 0.42              |
| 1:A:617:LYS:HA    | 1:A:617:LYS:HD3   | 1.80                     | 0.42              |
| 1:B:61:MET:HG3    | 1:B:67:ALA:HA     | 2.01                     | 0.42              |
| 1:A:2:GLY:N       | 1:A:187:ASP:OD2   | 2.53                     | 0.42              |
| 1:B:566:ALA:O     | 1:B:570:LEU:HB2   | 2.19                     | 0.42              |
| 1:A:584:LYS:HA    | 1:A:587:ILE:HD12  | 2.02                     | 0.41              |
| 1:B:238:LYS:HG3   | 1:B:238:LYS:HZ2   | 1.63                     | 0.41              |
| 1:A:24:VAL:CG1    | 1:B:881:MET:HE1   | 2.50                     | 0.41              |
| 1:B:87:SER:HA     | 1:B:129:ASP:HB3   | 2.01                     | 0.41              |
| 1:B:779:GLU:HB3   | 1:B:783:ARG:HH12  | 1.86                     | 0.41              |
| 1:A:717:ALA:HA    | 1:A:718:PRO:HD3   | 1.91                     | 0.41              |
| 1:B:750:ASN:HD21  | 1:B:1083:SER:HB2  | 1.86                     | 0.41              |
| 1:B:874:GLU:CD    | 7:B:4242:HOH:O    | 2.58                     | 0.41              |
| 1:A:507:GLY:N     | 1:A:537:LYS:O     | 2.51                     | 0.41              |
| 1:A:976:HIS:CE1   | 1:B:61:MET:HA     | 2.56                     | 0.41              |
| 1:A:1229:ARG:HH12 | 1:B:765:GLN:NE2   | 2.18                     | 0.41              |
| 1:A:24:VAL:HG13   | 1:B:881:MET:HE1   | 2.03                     | 0.41              |
| 1:A:289:HIS:HE1   | 7:A:3078:HOH:O    | 2.03                     | 0.41              |
| 1:B:1026:ALA:O    | 1:B:1030:MET:HG3  | 2.20                     | 0.41              |
| 1:A:233:ASN:HD21  | 1:B:331:LYS:HE3   | 1.84                     | 0.41              |
| 1:A:289:HIS:HD2   | 7:A:2635:HOH:O    | 2.03                     | 0.41              |
| 1:A:1174:SER:HB2  | 1:B:1154:HIS:HE1  | 1.86                     | 0.41              |
| 1:B:12:THR:CG2    | 1:B:39:GLU:OE2    | 2.69                     | 0.41              |
| 1:B:737:ARG:HH11  | 1:B:739:GLN:HE22  | 1.68                     | 0.41              |
| 1:B:569:LYS:HG2   | 1:B:570:LEU:HD13  | 2.02                     | 0.41              |
| 1:B:934:LEU:HD22  | 1:B:942:LEU:HG    | 2.03                     | 0.41              |
| 1:B:754:ILE:HD13  | 1:B:1084:GLN:HB2  | 2.02                     | 0.41              |
| 1:A:909:ALA:HB1   | 1:A:930:LEU:HD13  | 2.01                     | 0.41              |
| 1:A:1118:LYS:HE3  | 7:A:2370:HOH:O    | 2.21                     | 0.41              |
| 5:B:3236:HTL:H351 | 5:B:3236:HTL:H4A3 | 1.90                     | 0.41              |
| 5:A:2236:HTL:H5A1 | 5:A:2236:HTL:H4A1 | 1.56                     | 0.41              |
| 5:A:2236:HTL:C1'  | 6:A:2240:CO2:C    | 2.99                     | 0.41              |
| 1:B:184:GLU:HG2   | 1:B:185:VAL:N     | 2.36                     | 0.41              |
| 1:B:7:THR:OG1     | 1:B:439:LYS:HE3   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:35:THR:O     | 1:A:39:GLU:HG3    | 2.21                     | 0.41              |
| 1:B:1176:ALA:HA  | 1:B:1177:PRO:HD3  | 1.90                     | 0.41              |
| 1:A:20:ALA:HB2   | 1:A:188:TYR:CE1   | 2.56                     | 0.41              |
| 1:B:667:LEU:HB3  | 1:B:854:LYS:HA    | 2.01                     | 0.41              |
| 1:A:49:LYS:HE3   | 7:A:2963:HOH:O    | 2.21                     | 0.41              |
| 1:B:108:VAL:HG21 | 1:B:157:HIS:HA    | 2.02                     | 0.41              |
| 1:B:637:GLU:CG   | 1:B:638:PHE:N     | 2.84                     | 0.41              |
| 1:B:765:GLN:HE21 | 1:B:765:GLN:HA    | 1.86                     | 0.41              |
| 1:B:426:GLY:O    | 1:B:427:ALA:HB3   | 2.21                     | 0.41              |
| 1:B:576:PHE:HA   | 7:B:4071:HOH:O    | 2.21                     | 0.41              |
| 1:B:635:THR:HG21 | 7:B:4182:HOH:O    | 2.21                     | 0.41              |
| 1:A:822:ARG:HD3  | 7:A:2300:HOH:O    | 2.21                     | 0.40              |
| 1:A:784:ILE:HA   | 1:A:785:PRO:HD3   | 1.90                     | 0.40              |
| 7:A:2543:HOH:O   | 1:B:1200:THR:HG21 | 2.20                     | 0.40              |
| 1:A:764:MET:C    | 1:A:765:GLN:HG2   | 2.41                     | 0.40              |
| 1:A:491:ASN:HA   | 1:A:492:PRO:HD2   | 1.83                     | 0.40              |
| 1:A:667:LEU:HB3  | 1:A:854:LYS:HA    | 2.02                     | 0.40              |
| 1:A:730:GLU:CD   | 1:A:730:GLU:H     | 2.24                     | 0.40              |
| 1:A:229:ARG:HD2  | 7:B:3789:HOH:O    | 2.20                     | 0.40              |
| 1:B:781:ALA:HA   | 1:B:784:ILE:HD12  | 2.02                     | 0.40              |
| 1:A:250:VAL:HG12 | 7:A:2605:HOH:O    | 2.22                     | 0.40              |
| 1:B:16:HIS:HE1   | 1:B:186:LEU:O     | 2.05                     | 0.40              |
| 1:A:671:GLN:NE2  | 1:A:854:LYS:HD2   | 2.36                     | 0.40              |
| 1:B:840:CYS:SG   | 1:B:996:ASN:HB2   | 2.62                     | 0.40              |
| 1:B:869:PHE:CE2  | 1:B:969:ILE:HG21  | 2.57                     | 0.40              |
| 1:B:1076:LEU:HB3 | 7:B:4233:HOH:O    | 2.22                     | 0.40              |
| 1:A:283:ILE:HG21 | 1:A:299:LEU:HD13  | 2.04                     | 0.40              |
| 1:A:705:LEU:HA   | 1:A:706:PRO:HD3   | 1.95                     | 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     | 1229/1231 (100%) | 1181 (96%) | 42 (3%) | 6 (0%)   | 34          | 21 |
| 1   | B     | 1229/1231 (100%) | 1191 (97%) | 33 (3%) | 5 (0%)   | 39          | 27 |
| All | All   | 2458/2462 (100%) | 2372 (96%) | 75 (3%) | 11 (0%)  | 39          | 27 |

All (11) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 357  | LYS  |
| 1   | B     | 732  | LYS  |
| 1   | B     | 1178 | ALA  |
| 1   | A     | 732  | LYS  |
| 1   | A     | 1178 | ALA  |
| 1   | A     | 1181 | LYS  |
| 1   | B     | 1181 | LYS  |
| 1   | B     | 1231 | LYS  |
| 1   | A     | 1231 | LYS  |
| 1   | A     | 631  | ALA  |
| 1   | B     | 357  | LYS  |

### 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     | 978/978 (100%)   | 856 (88%)  | 122 (12%) | 6           | 2 |
| 1   | B     | 978/978 (100%)   | 873 (89%)  | 105 (11%) | 8           | 3 |
| All | All   | 1956/1956 (100%) | 1729 (88%) | 227 (12%) | 7           | 2 |

All (227) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | LYS  |
| 1   | A     | 8   | THR  |
| 1   | A     | 12  | THR  |
| 1   | A     | 14  | THR  |
| 1   | A     | 27  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 82  | THR  |
| 1   | A     | 141 | LEU  |
| 1   | A     | 154 | LEU  |
| 1   | A     | 180 | ILE  |
| 1   | A     | 181 | GLN  |
| 1   | A     | 184 | GLU  |
| 1   | A     | 194 | LEU  |
| 1   | A     | 198 | LYS  |
| 1   | A     | 204 | ARG  |
| 1   | A     | 215 | VAL  |
| 1   | A     | 226 | PHE  |
| 1   | A     | 227 | GLN  |
| 1   | A     | 239 | VAL  |
| 1   | A     | 245 | GLU  |
| 1   | A     | 260 | LEU  |
| 1   | A     | 264 | VAL  |
| 1   | A     | 290 | LEU  |
| 1   | A     | 317 | LEU  |
| 1   | A     | 324 | ILE  |
| 1   | A     | 325 | THR  |
| 1   | A     | 327 | LEU  |
| 1   | A     | 342 | LEU  |
| 1   | A     | 349 | VAL  |
| 1   | A     | 359 | LEU  |
| 1   | A     | 377 | SER  |
| 1   | A     | 392 | VAL  |
| 1   | A     | 398 | VAL  |
| 1   | A     | 403 | LEU  |
| 1   | A     | 415 | LYS  |
| 1   | A     | 439 | LYS  |
| 1   | A     | 456 | ASP  |
| 1   | A     | 463 | ILE  |
| 1   | A     | 465 | ILE  |
| 1   | A     | 491 | ASN  |
| 1   | A     | 495 | VAL  |
| 1   | A     | 501 | LEU  |
| 1   | A     | 509 | THR  |
| 1   | A     | 511 | VAL  |
| 1   | A     | 518 | SER  |
| 1   | A     | 524 | LYS  |
| 1   | A     | 532 | ARG  |
| 1   | A     | 538 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 548 | LYS  |
| 1   | A     | 558 | ARG  |
| 1   | A     | 560 | ASN  |
| 1   | A     | 570 | LEU  |
| 1   | A     | 573 | VAL  |
| 1   | A     | 577 | GLU  |
| 1   | A     | 583 | LEU  |
| 1   | A     | 586 | SER  |
| 1   | A     | 593 | LYS  |
| 1   | A     | 594 | LYS  |
| 1   | A     | 612 | SER  |
| 1   | A     | 613 | LEU  |
| 1   | A     | 621 | SER  |
| 1   | A     | 623 | LYS  |
| 1   | A     | 630 | LYS  |
| 1   | A     | 632 | GLU  |
| 1   | A     | 634 | MET  |
| 1   | A     | 635 | THR  |
| 1   | A     | 637 | GLU  |
| 1   | A     | 643 | VAL  |
| 1   | A     | 654 | LEU  |
| 1   | A     | 710 | LYS  |
| 1   | A     | 714 | LEU  |
| 1   | A     | 720 | ASN  |
| 1   | A     | 727 | LYS  |
| 1   | A     | 729 | LYS  |
| 1   | A     | 732 | LYS  |
| 1   | A     | 741 | ASN  |
| 1   | A     | 754 | ILE  |
| 1   | A     | 758 | LYS  |
| 1   | A     | 765 | GLN  |
| 1   | A     | 768 | ASP  |
| 1   | A     | 783 | ARG  |
| 1   | A     | 789 | GLU  |
| 1   | A     | 805 | LEU  |
| 1   | A     | 808 | PHE  |
| 1   | A     | 813 | SER  |
| 1   | A     | 831 | ARG  |
| 1   | A     | 849 | PRO  |
| 1   | A     | 858 | LEU  |
| 1   | A     | 880 | ASN  |
| 1   | A     | 893 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 910  | LEU  |
| 1   | A     | 914  | LEU  |
| 1   | A     | 917  | LYS  |
| 1   | A     | 930  | LEU  |
| 1   | A     | 938  | LYS  |
| 1   | A     | 941  | LEU  |
| 1   | A     | 953  | THR  |
| 1   | A     | 989  | MET  |
| 1   | A     | 993  | VAL  |
| 1   | A     | 997  | THR  |
| 1   | A     | 1000 | GLN  |
| 1   | A     | 1047 | GLN  |
| 1   | A     | 1048 | GLN  |
| 1   | A     | 1064 | LEU  |
| 1   | A     | 1077 | ARG  |
| 1   | A     | 1082 | LYS  |
| 1   | A     | 1088 | ASN  |
| 1   | A     | 1104 | ARG  |
| 1   | A     | 1115 | LEU  |
| 1   | A     | 1124 | VAL  |
| 1   | A     | 1136 | VAL  |
| 1   | A     | 1137 | LEU  |
| 1   | A     | 1146 | LYS  |
| 1   | A     | 1170 | ASN  |
| 1   | A     | 1173 | GLU  |
| 1   | A     | 1181 | LYS  |
| 1   | A     | 1183 | ASP  |
| 1   | A     | 1196 | THR  |
| 1   | A     | 1200 | THR  |
| 1   | A     | 1219 | THR  |
| 1   | A     | 1225 | ASP  |
| 1   | A     | 1231 | LYS  |
| 1   | A     | 1232 | LYS  |
| 1   | B     | 12   | THR  |
| 1   | B     | 14   | THR  |
| 1   | B     | 27   | ILE  |
| 1   | B     | 48   | ARG  |
| 1   | B     | 82   | THR  |
| 1   | B     | 141  | LEU  |
| 1   | B     | 154  | LEU  |
| 1   | B     | 168  | MET  |
| 1   | B     | 180  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 181 | GLN  |
| 1   | B     | 194 | LEU  |
| 1   | B     | 198 | LYS  |
| 1   | B     | 211 | GLU  |
| 1   | B     | 215 | VAL  |
| 1   | B     | 226 | PHE  |
| 1   | B     | 227 | GLN  |
| 1   | B     | 260 | LEU  |
| 1   | B     | 264 | VAL  |
| 1   | B     | 290 | LEU  |
| 1   | B     | 296 | LYS  |
| 1   | B     | 303 | ARG  |
| 1   | B     | 311 | GLU  |
| 1   | B     | 317 | LEU  |
| 1   | B     | 324 | ILE  |
| 1   | B     | 325 | THR  |
| 1   | B     | 327 | LEU  |
| 1   | B     | 342 | LEU  |
| 1   | B     | 349 | VAL  |
| 1   | B     | 351 | ARG  |
| 1   | B     | 359 | LEU  |
| 1   | B     | 383 | SER  |
| 1   | B     | 392 | VAL  |
| 1   | B     | 403 | LEU  |
| 1   | B     | 439 | LYS  |
| 1   | B     | 465 | ILE  |
| 1   | B     | 472 | GLU  |
| 1   | B     | 483 | ARG  |
| 1   | B     | 491 | ASN  |
| 1   | B     | 501 | LEU  |
| 1   | B     | 509 | THR  |
| 1   | B     | 511 | VAL  |
| 1   | B     | 532 | ARG  |
| 1   | B     | 570 | LEU  |
| 1   | B     | 582 | LEU  |
| 1   | B     | 583 | LEU  |
| 1   | B     | 593 | LYS  |
| 1   | B     | 594 | LYS  |
| 1   | B     | 613 | LEU  |
| 1   | B     | 617 | LYS  |
| 1   | B     | 620 | ASP  |
| 1   | B     | 628 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 630  | LYS  |
| 1   | B     | 637  | GLU  |
| 1   | B     | 643  | VAL  |
| 1   | B     | 654  | LEU  |
| 1   | B     | 698  | VAL  |
| 1   | B     | 702  | SER  |
| 1   | B     | 710  | LYS  |
| 1   | B     | 714  | LEU  |
| 1   | B     | 720  | ASN  |
| 1   | B     | 725  | GLU  |
| 1   | B     | 729  | LYS  |
| 1   | B     | 732  | LYS  |
| 1   | B     | 741  | ASN  |
| 1   | B     | 754  | ILE  |
| 1   | B     | 758  | LYS  |
| 1   | B     | 765  | GLN  |
| 1   | B     | 768  | ASP  |
| 1   | B     | 779  | GLU  |
| 1   | B     | 783  | ARG  |
| 1   | B     | 789  | GLU  |
| 1   | B     | 805  | LEU  |
| 1   | B     | 813  | SER  |
| 1   | B     | 821  | VAL  |
| 1   | B     | 831  | ARG  |
| 1   | B     | 858  | LEU  |
| 1   | B     | 874  | GLU  |
| 1   | B     | 880  | ASN  |
| 1   | B     | 893  | LEU  |
| 1   | B     | 910  | LEU  |
| 1   | B     | 914  | LEU  |
| 1   | B     | 917  | LYS  |
| 1   | B     | 930  | LEU  |
| 1   | B     | 942  | LEU  |
| 1   | B     | 953  | THR  |
| 1   | B     | 993  | VAL  |
| 1   | B     | 1000 | GLN  |
| 1   | B     | 1047 | GLN  |
| 1   | B     | 1048 | GLN  |
| 1   | B     | 1064 | LEU  |
| 1   | B     | 1077 | ARG  |
| 1   | B     | 1104 | ARG  |
| 1   | B     | 1115 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1118 | LYS  |
| 1   | B     | 1124 | VAL  |
| 1   | B     | 1136 | VAL  |
| 1   | B     | 1137 | LEU  |
| 1   | B     | 1140 | SER  |
| 1   | B     | 1162 | GLU  |
| 1   | B     | 1170 | ASN  |
| 1   | B     | 1181 | LYS  |
| 1   | B     | 1196 | THR  |
| 1   | B     | 1200 | THR  |
| 1   | B     | 1225 | ASP  |
| 1   | B     | 1228 | LYS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | ASN  |
| 1   | A     | 16  | HIS  |
| 1   | A     | 46  | GLN  |
| 1   | A     | 110 | HIS  |
| 1   | A     | 128 | GLN  |
| 1   | A     | 135 | GLN  |
| 1   | A     | 147 | GLN  |
| 1   | A     | 164 | ASN  |
| 1   | A     | 169 | HIS  |
| 1   | A     | 181 | GLN  |
| 1   | A     | 212 | HIS  |
| 1   | A     | 220 | GLN  |
| 1   | A     | 221 | ASN  |
| 1   | A     | 227 | GLN  |
| 1   | A     | 233 | ASN  |
| 1   | A     | 289 | HIS  |
| 1   | A     | 389 | HIS  |
| 1   | A     | 421 | GLN  |
| 1   | A     | 434 | ASN  |
| 1   | A     | 467 | HIS  |
| 1   | A     | 491 | ASN  |
| 1   | A     | 513 | ASN  |
| 1   | A     | 560 | ASN  |
| 1   | A     | 588 | HIS  |
| 1   | A     | 602 | ASN  |
| 1   | A     | 688 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 691  | GLN  |
| 1   | A     | 693  | ASN  |
| 1   | A     | 720  | ASN  |
| 1   | A     | 739  | GLN  |
| 1   | A     | 741  | ASN  |
| 1   | A     | 750  | ASN  |
| 1   | A     | 765  | GLN  |
| 1   | A     | 774  | GLN  |
| 1   | A     | 777  | ASN  |
| 1   | A     | 836  | ASN  |
| 1   | A     | 860  | GLN  |
| 1   | A     | 866  | ASN  |
| 1   | A     | 880  | ASN  |
| 1   | A     | 918  | ASN  |
| 1   | A     | 976  | HIS  |
| 1   | A     | 1000 | GLN  |
| 1   | A     | 1048 | GLN  |
| 1   | A     | 1084 | GLN  |
| 1   | A     | 1088 | ASN  |
| 1   | A     | 1132 | ASN  |
| 1   | A     | 1154 | HIS  |
| 1   | A     | 1215 | ASN  |
| 1   | B     | 11   | ASN  |
| 1   | B     | 16   | HIS  |
| 1   | B     | 46   | GLN  |
| 1   | B     | 110  | HIS  |
| 1   | B     | 128  | GLN  |
| 1   | B     | 135  | GLN  |
| 1   | B     | 147  | GLN  |
| 1   | B     | 169  | HIS  |
| 1   | B     | 181  | GLN  |
| 1   | B     | 212  | HIS  |
| 1   | B     | 220  | GLN  |
| 1   | B     | 221  | ASN  |
| 1   | B     | 227  | GLN  |
| 1   | B     | 233  | ASN  |
| 1   | B     | 288  | ASN  |
| 1   | B     | 389  | HIS  |
| 1   | B     | 421  | GLN  |
| 1   | B     | 434  | ASN  |
| 1   | B     | 467  | HIS  |
| 1   | B     | 491  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 513  | ASN  |
| 1   | B     | 536  | ASN  |
| 1   | B     | 560  | ASN  |
| 1   | B     | 602  | ASN  |
| 1   | B     | 688  | ASN  |
| 1   | B     | 691  | GLN  |
| 1   | B     | 693  | ASN  |
| 1   | B     | 720  | ASN  |
| 1   | B     | 739  | GLN  |
| 1   | B     | 741  | ASN  |
| 1   | B     | 750  | ASN  |
| 1   | B     | 765  | GLN  |
| 1   | B     | 774  | GLN  |
| 1   | B     | 777  | ASN  |
| 1   | B     | 836  | ASN  |
| 1   | B     | 860  | GLN  |
| 1   | B     | 866  | ASN  |
| 1   | B     | 880  | ASN  |
| 1   | B     | 911  | GLN  |
| 1   | B     | 918  | ASN  |
| 1   | B     | 976  | HIS  |
| 1   | B     | 1000 | GLN  |
| 1   | B     | 1048 | GLN  |
| 1   | B     | 1084 | GLN  |
| 1   | B     | 1088 | ASN  |
| 1   | B     | 1108 | GLN  |
| 1   | B     | 1132 | ASN  |
| 1   | B     | 1154 | HIS  |
| 1   | B     | 1215 | 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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   | SF4  | A     | 2233 | 1    | 0,12,12      | 0.00 | -        | 0,24,24     | 0.00 | -        |
| 4   | SF4  | A     | 2234 | 1    | 0,12,12      | 0.00 | -        | 0,24,24     | 0.00 | -        |
| 4   | SF4  | A     | 2235 | 1    | 0,12,12      | 0.00 | -        | 0,24,24     | 0.00 | -        |
| 5   | HTL  | A     | 2236 | 2    | 22,30,30     | 3.60 | 11 (50%) | 33,45,45    | 4.05 | 8 (24%)  |
| 6   | CO2  | A     | 2240 | -    | 0,2,2        | 0.00 | -        | 0,1,1       | 0.00 | -        |
| 4   | SF4  | B     | 3233 | 1    | 0,12,12      | 0.00 | -        | 0,24,24     | 0.00 | -        |
| 4   | SF4  | B     | 3234 | 1    | 0,12,12      | 0.00 | -        | 0,24,24     | 0.00 | -        |
| 4   | SF4  | B     | 3235 | 1    | 0,12,12      | 0.00 | -        | 0,24,24     | 0.00 | -        |
| 5   | HTL  | B     | 3236 | 2    | 22,30,30     | 3.91 | 8 (36%)  | 33,45,45    | 4.20 | 8 (24%)  |
| 6   | CO2  | B     | 3240 | -    | 0,2,2        | 0.00 | -        | 0,1,1       | 0.00 | -        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 4   | SF4  | A     | 2233 | 1    | -       | 0/0/48/48  | 0/6/5/5 |
| 4   | SF4  | A     | 2234 | 1    | -       | 0/0/48/48  | 0/6/5/5 |
| 4   | SF4  | A     | 2235 | 1    | -       | 0/0/48/48  | 0/6/5/5 |
| 5   | HTL  | A     | 2236 | 2    | -       | 0/16/21/21 | 0/2/2/2 |
| 6   | CO2  | A     | 2240 | -    | -       | 0/0/0/0    | 0/0/0/0 |
| 4   | SF4  | B     | 3233 | 1    | -       | 0/0/48/48  | 0/6/5/5 |
| 4   | SF4  | B     | 3234 | 1    | -       | 0/0/48/48  | 0/6/5/5 |
| 4   | SF4  | B     | 3235 | 1    | -       | 0/0/48/48  | 0/6/5/5 |
| 5   | HTL  | B     | 3236 | 2    | -       | 0/16/21/21 | 0/2/2/2 |
| 6   | CO2  | B     | 3240 | -    | -       | 0/0/0/0    | 0/0/0/0 |

All (19) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5   | B     | 3236 | HTL  | C4A-C4  | -7.77 | 1.33        | 1.49     |
| 5   | B     | 3236 | HTL  | C5-S1   | -4.97 | 1.64        | 1.74     |
| 5   | B     | 3236 | HTL  | C4-N3   | -4.39 | 1.30        | 1.39     |
| 5   | A     | 2236 | HTL  | C4A-C4  | -3.20 | 1.42        | 1.49     |
| 5   | A     | 2236 | HTL  | C2A-C2' | -3.19 | 1.39        | 1.49     |
| 5   | B     | 3236 | HTL  | C4'-N4' | -2.68 | 1.27        | 1.34     |
| 5   | A     | 2236 | HTL  | P2-O22  | -2.48 | 1.45        | 1.54     |
| 5   | A     | 2236 | HTL  | P1-O13  | -2.11 | 1.45        | 1.54     |
| 5   | A     | 2236 | HTL  | C3'-C1' | 2.69  | 1.57        | 1.49     |
| 5   | B     | 3236 | HTL  | C5'-C4' | 3.35  | 1.50        | 1.42     |
| 5   | A     | 2236 | HTL  | C2'-N3' | 4.47  | 1.42        | 1.34     |
| 5   | A     | 2236 | HTL  | C4'-N4' | 4.60  | 1.45        | 1.34     |
| 5   | A     | 2236 | HTL  | C5'-C4' | 5.85  | 1.56        | 1.42     |
| 5   | B     | 3236 | HTL  | C6'-N1' | 6.46  | 1.48        | 1.34     |
| 5   | A     | 2236 | HTL  | C6'-N1' | 6.63  | 1.48        | 1.34     |
| 5   | B     | 3236 | HTL  | C2'-N1' | 7.46  | 1.47        | 1.34     |
| 5   | A     | 2236 | HTL  | C2'-N1' | 7.58  | 1.47        | 1.34     |
| 5   | A     | 2236 | HTL  | C4'-N3' | 7.76  | 1.47        | 1.35     |
| 5   | B     | 3236 | HTL  | C4'-N3' | 9.55  | 1.49        | 1.35     |

All (16) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 5   | B     | 3236 | HTL  | C5A-C5-C4   | -19.02 | 110.52      | 127.56   |
| 5   | A     | 2236 | HTL  | C5A-C5-C4   | -15.89 | 113.32      | 127.56   |
| 5   | A     | 2236 | HTL  | C5A-C5-S1   | -12.37 | 102.92      | 120.24   |
| 5   | B     | 3236 | HTL  | C5A-C5-S1   | -11.22 | 104.53      | 120.24   |
| 5   | A     | 2236 | HTL  | C4A-C4-C5   | -4.30  | 119.23      | 128.90   |
| 5   | B     | 3236 | HTL  | N1'-C2'-N3' | -2.62  | 120.76      | 125.60   |
| 5   | A     | 2236 | HTL  | N1'-C2'-N3' | -2.52  | 120.94      | 125.60   |
| 5   | B     | 3236 | HTL  | P1-O5G-C5B  | 2.02   | 133.02      | 121.50   |
| 5   | B     | 3236 | HTL  | C5-C4-N3    | 2.40   | 113.41      | 107.83   |
| 5   | A     | 2236 | HTL  | O22-P2-O21  | 3.55   | 122.01      | 110.58   |
| 5   | B     | 3236 | HTL  | O22-P2-O21  | 3.58   | 122.10      | 110.58   |
| 5   | A     | 2236 | HTL  | C2A-C2'-N1' | 3.63   | 121.39      | 117.03   |
| 5   | B     | 3236 | HTL  | C2A-C2'-N1' | 3.79   | 121.58      | 117.03   |
| 5   | A     | 2236 | HTL  | O5G-C5B-C5A | 4.00   | 126.04      | 109.30   |
| 5   | B     | 3236 | HTL  | O5G-C5B-C5A | 5.29   | 131.45      | 109.30   |
| 5   | A     | 2236 | HTL  | C4A-C4-N3   | 6.66   | 131.63      | 122.82   |

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

4 monomers are involved in 6 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5   | A     | 2236 | HTL  | 3       | 0            |
| 6   | A     | 2240 | CO2  | 1       | 0            |
| 5   | B     | 3236 | HTL  | 2       | 0            |
| 6   | B     | 3240 | CO2  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.