



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 01:13 PM EDT

PDB ID : 2PDA / pdb\_00002pda  
Title : CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN PYRUVATE-FERREDOXIN OXIDOREDUCTASE FROM DESULFOVIBRIO AFRICANUS AND PYRUVATE.  
Authors : Chabriere, E.; Charon, M.H.  
Deposited on : 1998-11-10  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

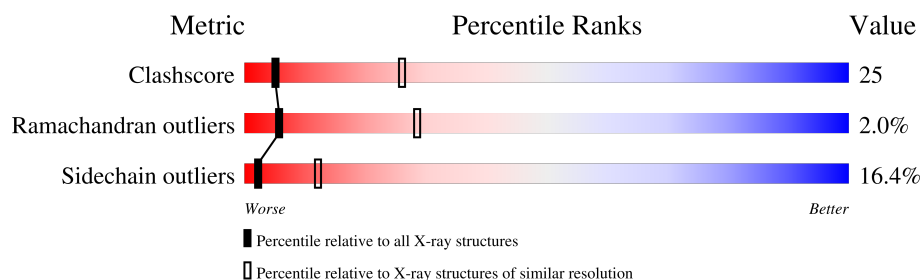
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 2977 (3.00-3.00)                                      |
| Ramachandran outliers | 187476                      | 2877 (3.00-3.00)                                      |
| Sidechain outliers    | 187428                      | 2880 (3.00-3.00)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 1231   |  |
| 1   | B     | 1231   |  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 4   | SF4  | A     | 1234 | -         | -        | X       | -                |
| 4   | SF4  | B     | 1241 | -         | -        | X       | -                |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18894 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 PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE).

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1231     | Total | C    | N    | O    | S  | 25      | 0       | 0     |
|     |       |          | 9382  | 5941 | 1599 | 1783 | 59 |         |         |       |
| 1   | B     | 1231     | Total | C    | N    | O    | S  | 25      | 0       | 0     |
|     |       |          | 9382  | 5941 | 1599 | 1783 | 59 |         |         |       |

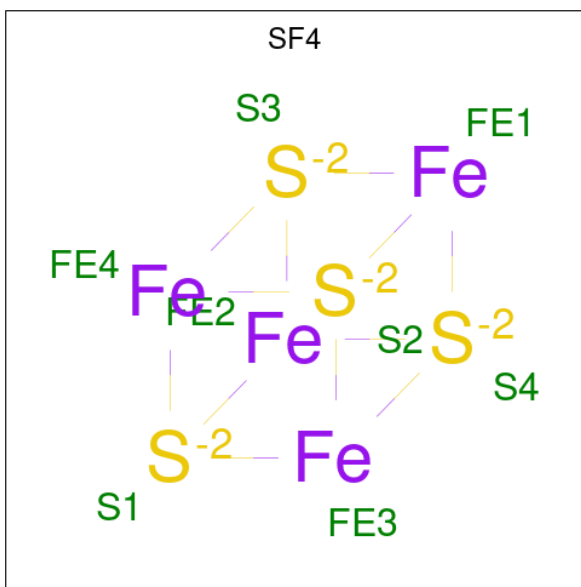
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

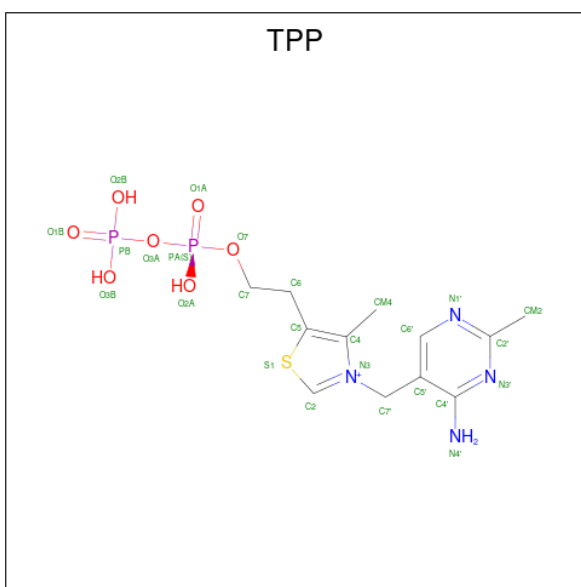
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | B     | 1        | Total | Ca | 0       | 0       |
|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

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



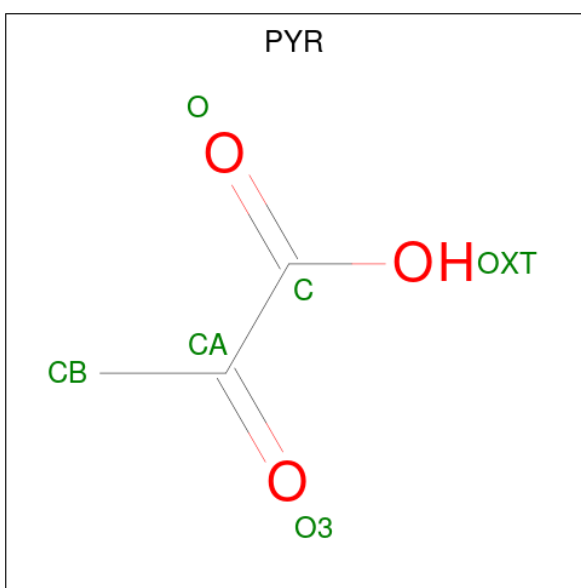
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 4   | A     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 8     | 4  | 4 |         |         |
| 4   | A     | 1        | Total | Fe | S | 0       | 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 THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



| Mol | Chain | Residues | Atoms       |         |        |        |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|--------|---------|---------|
| 5   | A     | 1        | Total<br>26 | C<br>12 | N<br>4 | O<br>7 | P<br>2 | S<br>1 | 0       | 0       |
| 5   | B     | 1        | Total<br>26 | C<br>12 | N<br>4 | O<br>7 | P<br>2 | S<br>1 | 0       | 0       |

- Molecule 6 is PYRUVIC ACID (CCD ID: PYR) (formula:  $\text{C}_3\text{H}_4\text{O}_3$ ).



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

- Molecule 7 is water.

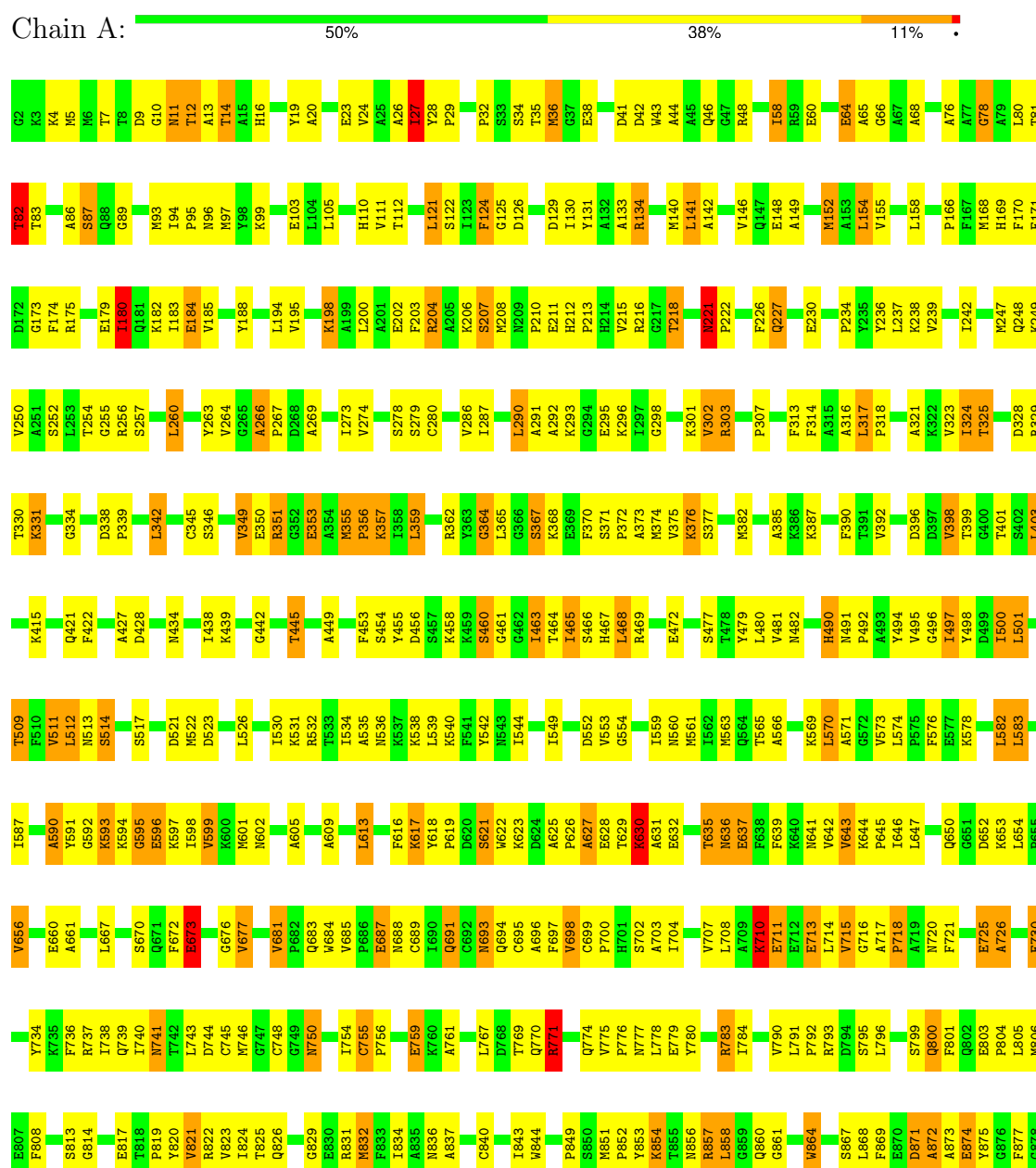
| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 7   | A     | 7        | Total<br>7 | O<br>7 | 0       | 0       |
| 7   | B     | 7        | Total<br>7 | O<br>7 | 0       | 0       |

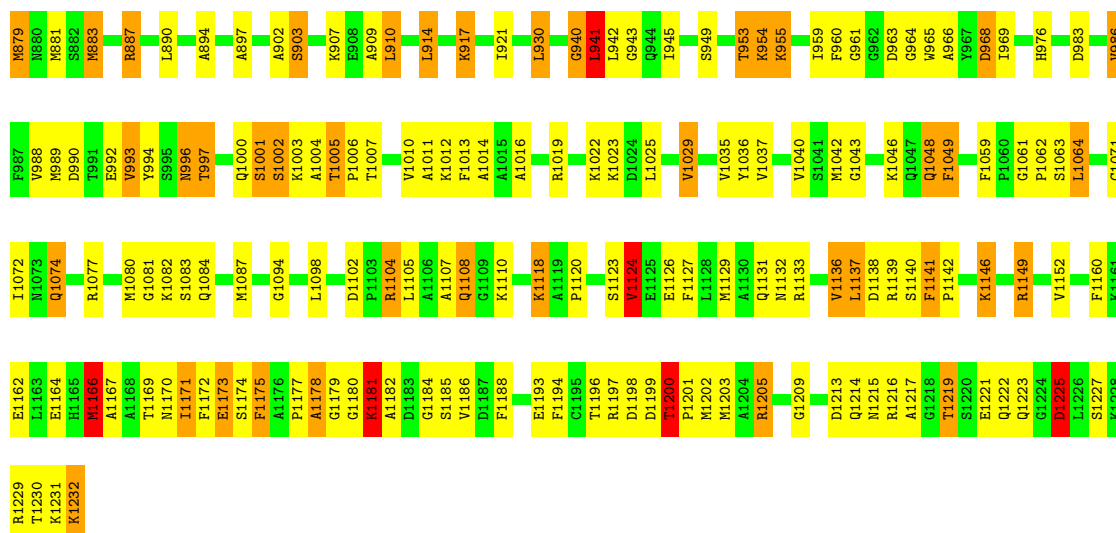
### 3 Residue-property plots

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

Note EDS was not executed.

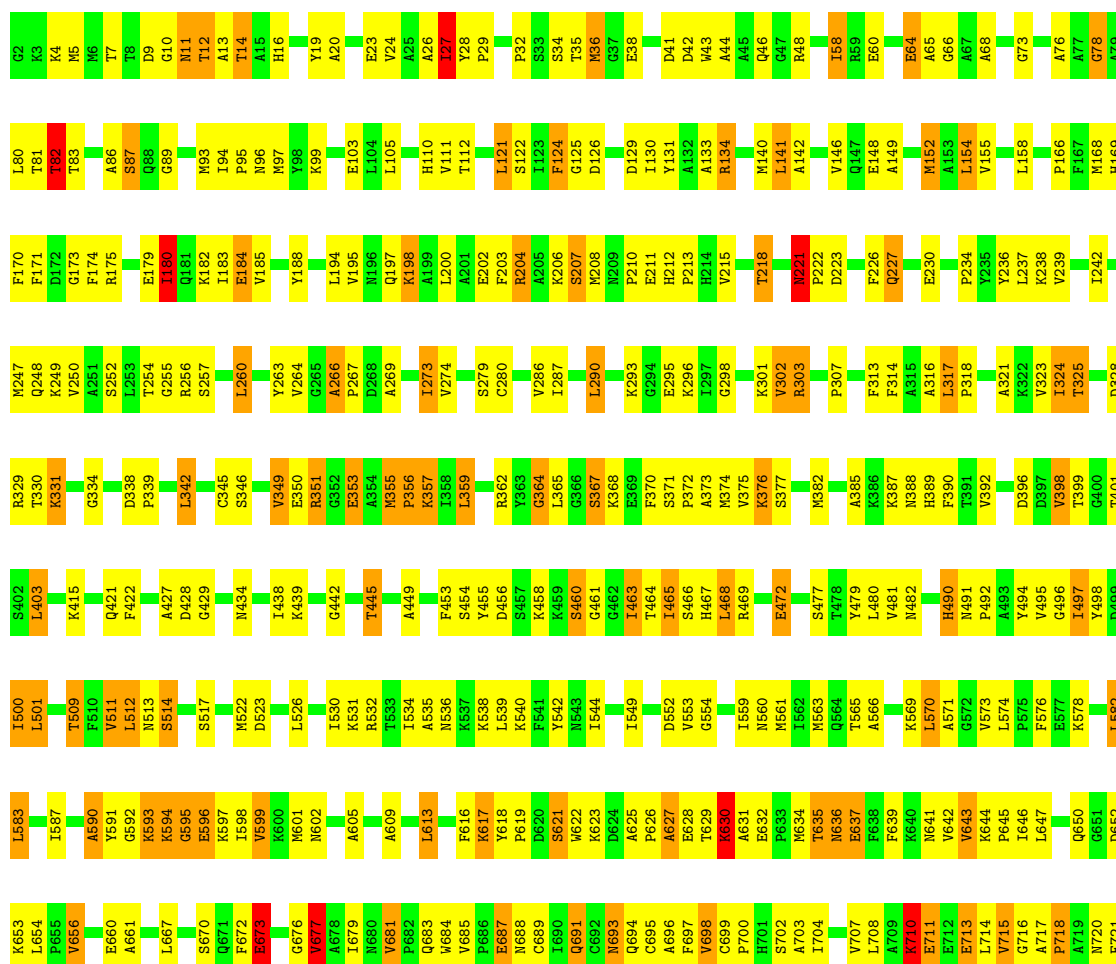
#### • Molecule 1: PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE)





• Molecule 1: PROTEIN (PYRUVATE-FERREDOXIN OXIDOREDUCTASE)

Chain B: 50% 38% 11% •



|       |       |       |      |      |      |
|-------|-------|-------|------|------|------|
| K1228 | R1149 | G1061 | H976 | E803 | E725 |
| R1229 | V1152 | P1062 | D983 | P804 | E726 |
| T1230 | F1160 | S1063 | V986 | L805 | A730 |
| K1231 | E1164 | L1064 | F987 | M806 | E730 |
| K1232 | H1165 | C1071 | M879 | F808 | Y734 |
|       | M1166 | I1072 | M880 | A811 | K735 |
|       | A1167 | N1073 | M881 | C812 | F736 |
|       | A1168 | Q1074 | M882 | S813 | R737 |
|       | T1169 | R1077 | M883 | G814 | I738 |
|       | N1170 | M1080 | R887 | E817 | Q739 |
|       | H1171 | G1081 | L890 | T818 | I740 |
|       | F1172 | K1082 | L893 | P819 | M741 |
|       | E1173 | S1083 | A894 | Y820 | I742 |
|       | S1174 | Q1084 | A897 | R821 | D744 |
|       | F1175 | M1087 | A902 | V823 | C745 |
|       | A1176 | G1087 | S903 | I824 | M746 |
|       | P1177 | S1000 | K907 | T825 | G747 |
|       | A1178 | S1001 | E908 | G829 | C748 |
|       | G1179 | S1002 | A909 | E830 | M750 |
|       | G1180 | K1003 | L910 | R831 | I754 |
|       | K1181 | A1004 | L914 | C755 | P756 |
|       | A1182 | T1005 | K917 | E759 | K760 |
|       | D1183 | P1006 | I921 | A761 | A761 |
|       | G1184 | T1007 | L930 | L767 | L767 |
|       | S1185 | V1010 | G940 | Q770 | Q770 |
|       | V1186 | A1011 | L941 | R771 | R771 |
|       | D1187 | K1012 | G943 | Q774 | Q774 |
|       | F1188 | F1013 | Q944 | V775 | V775 |
|       | E1189 | A1014 | I945 | N777 | N777 |
|       | F1194 | A1015 | S949 | L778 | L778 |
|       | C1195 | A1016 | T953 | E779 | E779 |
|       | T1196 | R1019 | K954 | Y780 | Y780 |
|       | R1197 | K1022 | K955 | R783 | R783 |
|       | D1198 | K1023 | I959 | I784 | I784 |
|       | D1199 | D1024 | F960 | V790 | V790 |
|       | T1200 | L1025 | G961 | L791 | L791 |
|       | P1201 | L1026 | N864 | P792 | P792 |
|       | M1202 | V1029 | G962 | R793 | R793 |
|       | M1203 | M1035 | D963 | D794 | D794 |
|       | A1204 | Y1036 | G964 | S795 | S795 |
|       | R1205 | V1037 | W965 | L796 | L796 |
|       | D1213 | M1042 | A966 | S799 | S799 |
|       | Q1214 | S1041 | T967 | Q800 | Q800 |
|       | N1215 | M1043 | D968 | A871 | A871 |
|       | R1216 | G1043 | I969 | A873 | A873 |
|       | T1219 | K1046 |      |      |      |
|       | S1220 | Q1047 |      |      |      |
|       | E1221 | Q1048 |      |      |      |
|       | Q1222 | F1049 |      |      |      |
|       | Q1223 | F1059 |      |      |      |
|       | G1224 | P1060 |      |      |      |
|       | D1225 |       |      |      |      |
|       | L1226 |       |      |      |      |
|       | S1227 |       |      |      |      |

## 4 Data and refinement statistics

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

| Property                                                 | Value                                          | Source    |
|----------------------------------------------------------|------------------------------------------------|-----------|
| Space group                                              | P 21 21 21                                     | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 86.00Å 146.30Å 211.90Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 10.00 – 3.00                                   | Depositor |
| % Data completeness<br>(in resolution range)             | 94.2 (10.00-3.00)                              | Depositor |
| $R_{merge}$                                              | (Not available)                                | Depositor |
| $R_{sym}$                                                | 0.10                                           | Depositor |
| Refinement program                                       | X-PLOR 3.854                                   | Depositor |
| R, $R_{free}$                                            | 0.234 , 0.297                                  | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtriage   |
| Total number of atoms                                    | 18894                                          | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 12.0                                           | 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: PYR, TPP, CA, MG, SF4

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     | 0.85         | 7/9584 (0.1%)   | 1.30        | 116/12954 (0.9%) |
| 1   | B     | 0.85         | 7/9584 (0.1%)   | 1.30        | 115/12954 (0.9%) |
| All | All   | 0.85         | 14/19168 (0.1%) | 1.30        | 231/25908 (0.9%) |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 879 | MET  | SD-CE | -6.70 | 1.62        | 1.79     |
| 1   | A     | 879 | MET  | SD-CE | -6.68 | 1.62        | 1.79     |
| 1   | A     | 953 | THR  | CA-CB | 6.13  | 1.62        | 1.53     |
| 1   | B     | 953 | THR  | CA-CB | 6.11  | 1.62        | 1.53     |
| 1   | A     | 36  | MET  | SD-CE | -5.86 | 1.64        | 1.79     |
| 1   | B     | 36  | MET  | SD-CE | -5.84 | 1.65        | 1.79     |
| 1   | B     | 94  | ILE  | CA-CB | 5.65  | 1.57        | 1.54     |
| 1   | A     | 94  | ILE  | CA-CB | 5.57  | 1.57        | 1.54     |
| 1   | A     | 872 | ALA  | CA-CB | -5.53 | 1.44        | 1.53     |
| 1   | B     | 872 | ALA  | CA-CB | -5.52 | 1.44        | 1.53     |
| 1   | A     | 180 | ILE  | CA-CB | 5.15  | 1.60        | 1.54     |
| 1   | B     | 180 | ILE  | CA-CB | 5.12  | 1.60        | 1.54     |
| 1   | B     | 302 | VAL  | CA-CB | 5.08  | 1.61        | 1.54     |
| 1   | A     | 302 | VAL  | CA-CB | 5.08  | 1.61        | 1.54     |

All (231) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | B     | 497 | ILE  | N-CA-C | 13.25  | 125.44      | 111.00   |
| 1   | A     | 497 | ILE  | N-CA-C | 13.25  | 125.44      | 111.00   |
| 1   | B     | 592 | GLY  | N-CA-C | -10.99 | 99.05       | 115.32   |
| 1   | A     | 592 | GLY  | N-CA-C | -10.96 | 99.09       | 115.32   |
| 1   | B     | 756 | PRO  | N-CA-C | 10.96  | 124.08      | 110.70   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 756  | PRO  | N-CA-C | 10.93 | 124.04      | 110.70   |
| 1   | A     | 755  | CYS  | CA-C-N | 10.23 | 130.91      | 120.38   |
| 1   | A     | 755  | CYS  | C-N-CA | 10.23 | 130.91      | 120.38   |
| 1   | B     | 755  | CYS  | CA-C-N | 10.18 | 130.87      | 120.38   |
| 1   | B     | 755  | CYS  | C-N-CA | 10.18 | 130.87      | 120.38   |
| 1   | B     | 590  | ALA  | N-CA-C | -9.92 | 97.43       | 110.53   |
| 1   | A     | 590  | ALA  | N-CA-C | -9.90 | 97.47       | 110.53   |
| 1   | B     | 1005 | THR  | CA-C-N | 8.88  | 128.83      | 120.03   |
| 1   | B     | 1005 | THR  | C-N-CA | 8.88  | 128.83      | 120.03   |
| 1   | A     | 1005 | THR  | CA-C-N | 8.88  | 128.82      | 120.03   |
| 1   | A     | 1005 | THR  | C-N-CA | 8.88  | 128.82      | 120.03   |
| 1   | A     | 27   | ILE  | N-CA-C | 8.61  | 121.38      | 108.80   |
| 1   | B     | 27   | ILE  | N-CA-C | 8.60  | 121.35      | 108.80   |
| 1   | B     | 625  | ALA  | N-CA-C | -8.21 | 99.40       | 109.83   |
| 1   | A     | 625  | ALA  | N-CA-C | -8.17 | 99.45       | 109.83   |
| 1   | B     | 871  | ASP  | N-CA-C | 8.14  | 121.30      | 110.88   |
| 1   | A     | 871  | ASP  | N-CA-C | 8.12  | 121.28      | 110.88   |
| 1   | A     | 636  | ASN  | N-CA-C | 8.08  | 120.76      | 110.33   |
| 1   | B     | 65   | ALA  | N-CA-C | -8.07 | 101.23      | 112.45   |
| 1   | A     | 65   | ALA  | N-CA-C | -8.07 | 101.24      | 112.45   |
| 1   | B     | 636  | ASN  | N-CA-C | 8.06  | 120.73      | 110.33   |
| 1   | B     | 618  | TYR  | CA-C-N | 7.92  | 127.92      | 119.76   |
| 1   | B     | 618  | TYR  | C-N-CA | 7.92  | 127.92      | 119.76   |
| 1   | A     | 618  | TYR  | CA-C-N | 7.90  | 127.90      | 119.76   |
| 1   | A     | 618  | TYR  | C-N-CA | 7.90  | 127.90      | 119.76   |
| 1   | A     | 1166 | MET  | N-CA-C | -7.68 | 94.45       | 110.80   |
| 1   | B     | 1166 | MET  | N-CA-C | -7.67 | 94.45       | 110.80   |
| 1   | A     | 641  | ASN  | N-CA-C | 7.62  | 122.68      | 113.23   |
| 1   | B     | 641  | ASN  | N-CA-C | 7.62  | 122.67      | 113.23   |
| 1   | B     | 1061 | GLY  | CA-C-N | 7.54  | 127.55      | 119.78   |
| 1   | B     | 1061 | GLY  | C-N-CA | 7.54  | 127.55      | 119.78   |
| 1   | A     | 1061 | GLY  | CA-C-N | 7.53  | 127.54      | 119.78   |
| 1   | A     | 1061 | GLY  | C-N-CA | 7.53  | 127.54      | 119.78   |
| 1   | A     | 355  | MET  | CA-C-N | 7.44  | 129.14      | 119.84   |
| 1   | A     | 355  | MET  | C-N-CA | 7.44  | 129.14      | 119.84   |
| 1   | B     | 355  | MET  | CA-C-N | 7.44  | 129.14      | 119.84   |
| 1   | B     | 355  | MET  | C-N-CA | 7.44  | 129.14      | 119.84   |
| 1   | B     | 125  | GLY  | N-CA-C | 7.40  | 125.74      | 111.31   |
| 1   | A     | 125  | GLY  | N-CA-C | 7.40  | 125.74      | 111.31   |
| 1   | B     | 909  | ALA  | N-CA-C | -7.38 | 102.83      | 111.03   |
| 1   | A     | 909  | ALA  | N-CA-C | -7.36 | 102.86      | 111.03   |
| 1   | B     | 203  | PHE  | N-CA-C | -7.29 | 103.34      | 111.28   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 203  | PHE  | N-CA-C | -7.29 | 103.34      | 111.28   |
| 1   | A     | 635  | THR  | N-CA-C | -7.18 | 98.10       | 109.23   |
| 1   | B     | 635  | THR  | N-CA-C | -7.16 | 98.13       | 109.23   |
| 1   | B     | 559  | ILE  | N-CA-C | 7.13  | 121.81      | 112.76   |
| 1   | A     | 877  | PHE  | N-CA-C | -7.13 | 104.39      | 113.23   |
| 1   | A     | 559  | ILE  | N-CA-C | 7.11  | 121.78      | 112.76   |
| 1   | B     | 877  | PHE  | N-CA-C | -7.10 | 104.43      | 113.23   |
| 1   | A     | 26   | ALA  | N-CA-C | -7.10 | 97.67       | 109.24   |
| 1   | B     | 26   | ALA  | N-CA-C | -7.07 | 97.72       | 109.24   |
| 1   | A     | 560  | ASN  | N-CA-C | 7.04  | 119.55      | 111.11   |
| 1   | B     | 560  | ASN  | N-CA-C | 7.03  | 119.55      | 111.11   |
| 1   | B     | 627  | ALA  | N-CA-C | 7.03  | 125.77      | 110.80   |
| 1   | A     | 627  | ALA  | N-CA-C | 7.00  | 125.72      | 110.80   |
| 1   | B     | 1200 | THR  | CA-C-N | 6.95  | 127.09      | 119.87   |
| 1   | B     | 1200 | THR  | C-N-CA | 6.95  | 127.09      | 119.87   |
| 1   | A     | 1200 | THR  | CA-C-N | 6.93  | 127.08      | 119.87   |
| 1   | A     | 1200 | THR  | C-N-CA | 6.93  | 127.08      | 119.87   |
| 1   | B     | 1014 | ALA  | N-CA-C | -6.91 | 102.45      | 111.71   |
| 1   | A     | 625  | ALA  | CA-C-N | -6.91 | 111.20      | 119.84   |
| 1   | A     | 625  | ALA  | C-N-CA | -6.91 | 111.20      | 119.84   |
| 1   | A     | 1014 | ALA  | N-CA-C | -6.91 | 102.46      | 111.71   |
| 1   | A     | 207  | SER  | N-CA-C | 6.89  | 118.88      | 110.41   |
| 1   | B     | 16   | HIS  | N-CA-C | -6.89 | 103.46      | 110.97   |
| 1   | B     | 207  | SER  | N-CA-C | 6.88  | 118.88      | 110.41   |
| 1   | A     | 711  | GLU  | N-CA-C | 6.88  | 125.45      | 110.80   |
| 1   | A     | 16   | HIS  | N-CA-C | -6.87 | 103.48      | 110.97   |
| 1   | B     | 625  | ALA  | CA-C-N | -6.87 | 111.25      | 119.84   |
| 1   | B     | 625  | ALA  | C-N-CA | -6.87 | 111.25      | 119.84   |
| 1   | B     | 711  | GLU  | N-CA-C | 6.86  | 125.41      | 110.80   |
| 1   | B     | 195  | VAL  | N-CA-C | 6.79  | 117.80      | 108.84   |
| 1   | A     | 195  | VAL  | N-CA-C | 6.78  | 117.80      | 108.84   |
| 1   | B     | 124  | PHE  | N-CA-C | 6.76  | 118.58      | 110.19   |
| 1   | A     | 124  | PHE  | N-CA-C | 6.75  | 118.56      | 110.19   |
| 1   | B     | 221  | ASN  | CA-C-N | -6.75 | 112.83      | 119.64   |
| 1   | B     | 221  | ASN  | C-N-CA | -6.75 | 112.83      | 119.64   |
| 1   | B     | 1175 | PHE  | N-CA-C | 6.74  | 120.27      | 108.75   |
| 1   | A     | 1175 | PHE  | N-CA-C | 6.73  | 120.26      | 108.75   |
| 1   | A     | 221  | ASN  | CA-C-N | -6.71 | 112.86      | 119.64   |
| 1   | A     | 221  | ASN  | C-N-CA | -6.71 | 112.86      | 119.64   |
| 1   | A     | 824  | ILE  | N-CA-C | -6.64 | 104.01      | 110.72   |
| 1   | B     | 824  | ILE  | N-CA-C | -6.64 | 104.02      | 110.72   |
| 1   | A     | 685  | VAL  | CA-C-N | 6.63  | 126.88      | 119.32   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 685  | VAL  | C-N-CA | 6.63  | 126.88      | 119.32   |
| 1   | B     | 685  | VAL  | CA-C-N | 6.61  | 126.85      | 119.32   |
| 1   | B     | 685  | VAL  | C-N-CA | 6.61  | 126.85      | 119.32   |
| 1   | B     | 247  | MET  | N-CA-C | -6.60 | 104.11      | 111.71   |
| 1   | A     | 247  | MET  | N-CA-C | -6.60 | 104.12      | 111.71   |
| 1   | B     | 1072 | ILE  | N-CA-C | -6.46 | 104.19      | 110.72   |
| 1   | A     | 1072 | ILE  | N-CA-C | -6.45 | 104.21      | 110.72   |
| 1   | A     | 1049 | PHE  | N-CA-C | -6.36 | 104.27      | 111.14   |
| 1   | B     | 1049 | PHE  | N-CA-C | -6.32 | 104.31      | 111.14   |
| 1   | B     | 759  | GLU  | N-CA-C | -6.32 | 96.87       | 107.99   |
| 1   | A     | 759  | GLU  | N-CA-C | -6.31 | 96.88       | 107.99   |
| 1   | A     | 66   | GLY  | N-CA-C | -6.31 | 105.18      | 112.50   |
| 1   | B     | 66   | GLY  | N-CA-C | -6.29 | 105.20      | 112.50   |
| 1   | B     | 29   | PRO  | N-CA-C | 6.25  | 120.31      | 110.50   |
| 1   | A     | 29   | PRO  | N-CA-C | 6.20  | 120.24      | 110.50   |
| 1   | A     | 1140 | SER  | N-CA-C | 6.17  | 120.81      | 113.28   |
| 1   | B     | 1140 | SER  | N-CA-C | 6.15  | 120.78      | 113.28   |
| 1   | A     | 500  | ILE  | N-CA-C | 6.15  | 117.63      | 110.62   |
| 1   | B     | 500  | ILE  | N-CA-C | 6.14  | 117.62      | 110.62   |
| 1   | A     | 637  | GLU  | N-CA-C | -6.13 | 104.66      | 111.71   |
| 1   | B     | 637  | GLU  | N-CA-C | -6.13 | 104.66      | 111.71   |
| 1   | B     | 708  | LEU  | N-CA-C | -6.12 | 97.22       | 107.80   |
| 1   | A     | 708  | LEU  | N-CA-C | -6.11 | 97.22       | 107.80   |
| 1   | A     | 364  | GLY  | N-CA-C | 6.06  | 127.55      | 113.18   |
| 1   | B     | 364  | GLY  | N-CA-C | 6.06  | 127.54      | 113.18   |
| 1   | B     | 376  | LYS  | N-CA-C | -6.03 | 104.70      | 111.28   |
| 1   | A     | 376  | LYS  | N-CA-C | -6.00 | 104.74      | 111.28   |
| 1   | A     | 501  | LEU  | N-CA-C | 5.97  | 119.52      | 112.72   |
| 1   | B     | 501  | LEU  | N-CA-C | 5.95  | 119.51      | 112.72   |
| 1   | A     | 618  | TYR  | N-CA-C | 5.93  | 119.24      | 109.58   |
| 1   | B     | 618  | TYR  | N-CA-C | 5.90  | 119.20      | 109.58   |
| 1   | A     | 1046 | LYS  | N-CA-C | -5.86 | 105.97      | 113.23   |
| 1   | B     | 1046 | LYS  | N-CA-C | -5.84 | 105.99      | 113.23   |
| 1   | A     | 832  | MET  | N-CA-C | 5.81  | 119.01      | 109.72   |
| 1   | B     | 832  | MET  | N-CA-C | 5.79  | 118.99      | 109.72   |
| 1   | A     | 997  | THR  | N-CA-C | 5.78  | 120.48      | 113.38   |
| 1   | A     | 673  | GLU  | N-CA-C | 5.76  | 118.43      | 111.40   |
| 1   | B     | 997  | THR  | N-CA-C | 5.76  | 120.47      | 113.38   |
| 1   | B     | 673  | GLU  | N-CA-C | 5.75  | 118.42      | 111.40   |
| 1   | A     | 1081 | GLY  | N-CA-C | -5.73 | 105.69      | 113.37   |
| 1   | A     | 861  | GLY  | CA-C-N | 5.71  | 126.60      | 119.98   |
| 1   | A     | 861  | GLY  | C-N-CA | 5.71  | 126.60      | 119.98   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | B     | 1081 | GLY  | N-CA-C  | -5.70 | 105.73      | 113.37   |
| 1   | B     | 1087 | MET  | N-CA-C  | -5.70 | 105.06      | 111.28   |
| 1   | B     | 861  | GLY  | CA-C-N  | 5.70  | 126.59      | 119.98   |
| 1   | B     | 861  | GLY  | C-N-CA  | 5.70  | 126.59      | 119.98   |
| 1   | B     | 630  | LYS  | N-CA-C  | 5.69  | 118.01      | 108.23   |
| 1   | B     | 490  | HIS  | N-CA-C  | 5.68  | 119.91      | 113.15   |
| 1   | A     | 1087 | MET  | N-CA-C  | -5.68 | 105.09      | 111.28   |
| 1   | A     | 630  | LYS  | N-CA-C  | 5.67  | 117.98      | 108.23   |
| 1   | B     | 750  | ASN  | N-CA-C  | 5.66  | 117.91      | 111.11   |
| 1   | A     | 750  | ASN  | N-CA-C  | 5.65  | 117.89      | 111.11   |
| 1   | A     | 78   | GLY  | N-CA-C  | 5.65  | 121.80      | 115.08   |
| 1   | B     | 78   | GLY  | N-CA-C  | 5.65  | 121.80      | 115.08   |
| 1   | A     | 490  | HIS  | N-CA-C  | 5.65  | 119.87      | 113.15   |
| 1   | B     | 385  | ALA  | N-CA-C  | 5.62  | 117.41      | 111.28   |
| 1   | A     | 652  | ASP  | N-CA-C  | -5.61 | 105.31      | 111.82   |
| 1   | B     | 652  | ASP  | N-CA-C  | -5.61 | 105.31      | 111.82   |
| 1   | A     | 385  | ALA  | N-CA-C  | 5.61  | 117.39      | 111.28   |
| 1   | B     | 13   | ALA  | N-CA-C  | -5.59 | 105.19      | 111.28   |
| 1   | A     | 983  | ASP  | N-CA-C  | 5.58  | 118.49      | 108.17   |
| 1   | B     | 983  | ASP  | N-CA-C  | 5.58  | 118.49      | 108.17   |
| 1   | A     | 13   | ALA  | N-CA-C  | -5.56 | 105.22      | 111.28   |
| 1   | A     | 313  | PHE  | N-CA-C  | -5.55 | 104.92      | 110.97   |
| 1   | B     | 1172 | PHE  | N-CA-C  | 5.54  | 116.88      | 108.07   |
| 1   | B     | 313  | PHE  | N-CA-C  | -5.53 | 104.94      | 110.97   |
| 1   | A     | 1172 | PHE  | N-CA-C  | 5.52  | 116.85      | 108.07   |
| 1   | B     | 631  | ALA  | N-CA-C  | -5.52 | 100.62      | 109.39   |
| 1   | A     | 631  | ALA  | N-CA-C  | -5.51 | 100.62      | 109.39   |
| 1   | B     | 255  | GLY  | N-CA-C  | -5.50 | 107.77      | 114.92   |
| 1   | A     | 255  | GLY  | N-CA-C  | -5.49 | 107.78      | 114.92   |
| 1   | A     | 968  | ASP  | N-CA-C  | 5.48  | 116.85      | 108.30   |
| 1   | B     | 968  | ASP  | N-CA-C  | 5.47  | 116.83      | 108.30   |
| 1   | A     | 713  | GLU  | N-CA-C  | -5.46 | 105.75      | 112.90   |
| 1   | A     | 27   | ILE  | N-CA-CB | -5.44 | 104.91      | 112.52   |
| 1   | B     | 713  | GLU  | N-CA-C  | -5.44 | 105.78      | 112.90   |
| 1   | A     | 1023 | LYS  | N-CA-C  | -5.43 | 101.81      | 109.96   |
| 1   | B     | 1023 | LYS  | N-CA-C  | -5.42 | 101.83      | 109.96   |
| 1   | B     | 27   | ILE  | N-CA-CB | -5.42 | 104.93      | 112.52   |
| 1   | A     | 771  | ARG  | N-CA-C  | 5.42  | 122.34      | 110.80   |
| 1   | B     | 774  | GLN  | N-CA-C  | 5.41  | 119.73      | 113.18   |
| 1   | B     | 771  | ARG  | N-CA-C  | 5.41  | 122.32      | 110.80   |
| 1   | B     | 571  | ALA  | N-CA-C  | 5.40  | 117.92      | 111.71   |
| 1   | A     | 774  | GLN  | N-CA-C  | 5.39  | 119.70      | 113.18   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | B     | 596  | GLU  | N-CA-C  | 5.38  | 116.96      | 111.14   |
| 1   | A     | 571  | ALA  | N-CA-C  | 5.38  | 117.89      | 111.71   |
| 1   | B     | 535  | ALA  | N-CA-C  | 5.37  | 119.37      | 111.04   |
| 1   | A     | 596  | GLU  | N-CA-C  | 5.37  | 116.94      | 111.14   |
| 1   | A     | 535  | ALA  | N-CA-C  | 5.35  | 119.33      | 111.04   |
| 1   | B     | 445  | THR  | N-CA-C  | -5.34 | 101.00      | 108.96   |
| 1   | A     | 725  | GLU  | N-CA-C  | -5.33 | 101.85      | 110.32   |
| 1   | A     | 445  | THR  | N-CA-C  | -5.33 | 101.03      | 108.96   |
| 1   | B     | 725  | GLU  | N-CA-C  | -5.32 | 101.86      | 110.32   |
| 1   | A     | 41   | ASP  | N-CA-C  | 5.29  | 118.20      | 111.69   |
| 1   | B     | 1225 | ASP  | N-CA-C  | -5.29 | 105.63      | 111.71   |
| 1   | A     | 266  | ALA  | N-CA-C  | 5.28  | 116.54      | 109.83   |
| 1   | A     | 1225 | ASP  | N-CA-C  | -5.28 | 105.64      | 111.71   |
| 1   | B     | 41   | ASP  | N-CA-C  | 5.28  | 118.18      | 111.69   |
| 1   | B     | 266  | ALA  | N-CA-C  | 5.26  | 116.52      | 109.83   |
| 1   | B     | 864  | TRP  | N-CA-C  | 5.26  | 118.06      | 109.59   |
| 1   | A     | 864  | TRP  | N-CA-C  | 5.26  | 118.06      | 109.59   |
| 1   | A     | 710  | LYS  | N-CA-C  | -5.26 | 102.50      | 110.28   |
| 1   | B     | 710  | LYS  | N-CA-C  | -5.25 | 102.50      | 110.28   |
| 1   | B     | 428  | ASP  | N-CA-C  | -5.23 | 106.30      | 113.30   |
| 1   | A     | 726  | ALA  | N-CA-C  | 5.22  | 117.24      | 109.25   |
| 1   | A     | 428  | ASP  | N-CA-C  | -5.22 | 106.31      | 113.30   |
| 1   | B     | 726  | ALA  | N-CA-C  | 5.22  | 117.23      | 109.25   |
| 1   | A     | 1171 | ILE  | CB-CA-C | -5.21 | 104.44      | 111.63   |
| 1   | A     | 1173 | GLU  | N-CA-C  | 5.19  | 116.76      | 108.41   |
| 1   | A     | 595  | GLY  | N-CA-C  | 5.18  | 125.47      | 113.18   |
| 1   | B     | 595  | GLY  | N-CA-C  | 5.18  | 125.45      | 113.18   |
| 1   | B     | 1173 | GLU  | N-CA-C  | 5.18  | 116.75      | 108.41   |
| 1   | B     | 1141 | PHE  | CA-C-N  | 5.18  | 124.63      | 119.24   |
| 1   | B     | 1141 | PHE  | C-N-CA  | 5.18  | 124.63      | 119.24   |
| 1   | B     | 1171 | ILE  | CB-CA-C | -5.18 | 104.48      | 111.63   |
| 1   | A     | 427  | ALA  | N-CA-C  | 5.17  | 118.85      | 112.24   |
| 1   | B     | 427  | ALA  | N-CA-C  | 5.14  | 118.82      | 112.24   |
| 1   | A     | 1141 | PHE  | CA-C-N  | 5.12  | 124.57      | 119.24   |
| 1   | A     | 1141 | PHE  | C-N-CA  | 5.12  | 124.57      | 119.24   |
| 1   | A     | 254  | THR  | N-CA-C  | 5.11  | 119.51      | 113.12   |
| 1   | B     | 254  | THR  | N-CA-C  | 5.11  | 119.51      | 113.12   |
| 1   | A     | 80   | LEU  | N-CA-C  | -5.10 | 102.14      | 110.20   |
| 1   | B     | 1167 | ALA  | N-CA-C  | -5.09 | 105.73      | 111.28   |
| 1   | A     | 616  | PHE  | N-CA-C  | -5.09 | 101.47      | 109.25   |
| 1   | B     | 80   | LEU  | N-CA-C  | -5.09 | 102.16      | 110.20   |
| 1   | B     | 155  | VAL  | CB-CA-C | -5.08 | 105.37      | 111.88   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 155  | VAL  | CB-CA-C | -5.08 | 105.38      | 111.88   |
| 1   | A     | 693  | ASN  | N-CA-C  | 5.07  | 118.77      | 112.58   |
| 1   | A     | 677  | VAL  | N-CA-C  | 5.07  | 117.77      | 112.90   |
| 1   | B     | 693  | ASN  | N-CA-C  | 5.07  | 118.76      | 112.58   |
| 1   | B     | 76   | ALA  | N-CA-C  | -5.07 | 105.03      | 111.11   |
| 1   | A     | 1167 | ALA  | N-CA-C  | -5.06 | 105.76      | 111.28   |
| 1   | B     | 616  | PHE  | N-CA-C  | -5.05 | 101.53      | 109.25   |
| 1   | B     | 677  | VAL  | N-CA-C  | 5.04  | 117.74      | 112.90   |
| 1   | A     | 76   | ALA  | N-CA-C  | -5.04 | 105.07      | 111.11   |
| 1   | A     | 82   | THR  | CB-CA-C | -5.03 | 99.45       | 110.67   |
| 1   | B     | 82   | THR  | CB-CA-C | -5.03 | 99.45       | 110.67   |
| 1   | A     | 836  | ASN  | N-CA-C  | 5.03  | 116.95      | 108.96   |
| 1   | B     | 836  | ASN  | N-CA-C  | 5.02  | 116.94      | 108.96   |
| 1   | A     | 769  | THR  | N-CA-C  | -5.01 | 107.17      | 113.28   |
| 1   | A     | 278  | SER  | N-CA-C  | 5.00  | 119.02      | 113.01   |
| 1   | B     | 594  | LYS  | N-CA-C  | -5.00 | 99.63       | 108.23   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 9382  | 0        | 9263     | 486     | 4            |
| 1   | B     | 9382  | 0        | 9263     | 489     | 4            |
| 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        | 4       | 0            |
| 4   | B     | 24    | 0        | 0        | 4       | 0            |
| 5   | A     | 26    | 0        | 16       | 6       | 0            |
| 5   | B     | 26    | 0        | 16       | 6       | 0            |
| 6   | A     | 6     | 0        | 0        | 2       | 0            |
| 6   | B     | 6     | 0        | 0        | 2       | 0            |
| 7   | A     | 7     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | B     | 7     | 0        | 0        | 0       | 0            |
| All | All   | 18894 | 0        | 18558    | 922     | 4            |

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 25.

All (922) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1184:GLY:HA3 | 1:B:1141:PHE:HZ   | 1.17                     | 1.08              |
| 1:B:805:LEU:HA   | 1:B:854:LYS:HZ2   | 1.17                     | 1.06              |
| 1:A:805:LEU:HA   | 1:A:854:LYS:HZ2   | 1.20                     | 1.05              |
| 1:A:124:PHE:HB3  | 1:A:367:SER:HB2   | 1.37                     | 1.04              |
| 1:B:124:PHE:HB3  | 1:B:367:SER:HB2   | 1.37                     | 1.02              |
| 1:A:68:ALA:HB2   | 1:A:93:MET:HG2    | 1.46                     | 0.97              |
| 1:B:68:ALA:HB2   | 1:B:93:MET:HG2    | 1.46                     | 0.97              |
| 1:A:1141:PHE:HZ  | 1:B:1184:GLY:HA3  | 1.31                     | 0.95              |
| 1:A:1184:GLY:HA3 | 1:B:1141:PHE:CZ   | 2.02                     | 0.94              |
| 1:A:805:LEU:HA   | 1:A:854:LYS:NZ    | 1.83                     | 0.92              |
| 1:B:805:LEU:HA   | 1:B:854:LYS:NZ    | 1.83                     | 0.92              |
| 1:B:1149:ARG:HG3 | 1:B:1149:ARG:HH11 | 1.36                     | 0.91              |
| 1:A:1149:ARG:HG3 | 1:A:1149:ARG:HH11 | 1.36                     | 0.90              |
| 1:A:1132:ASN:O   | 1:A:1136:VAL:HG22 | 1.75                     | 0.86              |
| 1:B:1132:ASN:O   | 1:B:1136:VAL:HG22 | 1.75                     | 0.86              |
| 1:B:639:PHE:HA   | 1:B:643:VAL:HG13  | 1.58                     | 0.85              |
| 1:B:832:MET:HE2  | 1:B:834:ILE:HD11  | 1.58                     | 0.85              |
| 1:A:832:MET:HE2  | 1:A:834:ILE:HD11  | 1.58                     | 0.85              |
| 1:B:554:GLY:HA3  | 1:B:601:MET:HE2   | 1.58                     | 0.85              |
| 1:A:9:ASP:OD1    | 1:A:12:THR:HG23   | 1.77                     | 0.84              |
| 1:B:9:ASP:OD1    | 1:B:12:THR:HG23   | 1.77                     | 0.84              |
| 1:A:492:PRO:O    | 1:A:495:VAL:HG12  | 1.78                     | 0.84              |
| 1:A:1000:GLN:HA  | 1:A:1012:LYS:HB2  | 1.60                     | 0.83              |
| 1:A:554:GLY:HA3  | 1:A:601:MET:HE2   | 1.58                     | 0.83              |
| 1:A:639:PHE:HA   | 1:A:643:VAL:HG13  | 1.58                     | 0.83              |
| 1:B:110:HIS:CD2  | 1:B:169:HIS:HD2   | 1.97                     | 0.82              |
| 1:B:1000:GLN:HA  | 1:B:1012:LYS:HB2  | 1.60                     | 0.82              |
| 1:B:99:LYS:O     | 1:B:103:GLU:HG3   | 1.79                     | 0.82              |
| 1:B:492:PRO:O    | 1:B:495:VAL:HG12  | 1.78                     | 0.82              |
| 1:A:110:HIS:CD2  | 1:A:169:HIS:HD2   | 1.97                     | 0.81              |
| 1:B:349:VAL:HA   | 1:B:355:MET:HE1   | 1.62                     | 0.81              |
| 1:A:99:LYS:O     | 1:A:103:GLU:HG3   | 1.79                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:130:ILE:HG13  | 1:A:131:TYR:N     | 1.95                     | 0.80              |
| 1:A:349:VAL:HA    | 1:A:355:MET:HE1   | 1.62                     | 0.80              |
| 1:A:688:ASN:ND2   | 1:A:759:GLU:HB2   | 1.97                     | 0.80              |
| 1:B:831:ARG:HD2   | 1:B:954:LYS:O     | 1.82                     | 0.80              |
| 1:A:1184:GLY:CA   | 1:B:1141:PHE:HZ   | 1.95                     | 0.80              |
| 1:B:544:ILE:HD12  | 1:B:613:LEU:HD13  | 1.63                     | 0.80              |
| 1:A:455:TYR:HB2   | 1:B:1201:PRO:HG3  | 1.63                     | 0.80              |
| 1:B:130:ILE:HG13  | 1:B:131:TYR:N     | 1.95                     | 0.79              |
| 1:A:831:ARG:HD2   | 1:A:954:LYS:O     | 1.82                     | 0.79              |
| 1:A:544:ILE:HD12  | 1:A:613:LEU:HD13  | 1.63                     | 0.79              |
| 1:B:688:ASN:ND2   | 1:B:759:GLU:HB2   | 1.97                     | 0.78              |
| 1:A:755:CYS:SG    | 1:A:761:ALA:HB3   | 2.23                     | 0.78              |
| 1:B:755:CYS:SG    | 1:B:761:ALA:HB3   | 2.23                     | 0.77              |
| 1:B:1132:ASN:HD21 | 1:B:1139:ARG:HH12 | 1.32                     | 0.77              |
| 1:A:1141:PHE:CZ   | 1:B:1184:GLY:HA3  | 2.18                     | 0.77              |
| 1:A:330:THR:O     | 1:A:362:ARG:HD3   | 1.84                     | 0.77              |
| 1:A:1132:ASN:HD21 | 1:A:1139:ARG:HH12 | 1.32                     | 0.77              |
| 1:B:739:GLN:HE22  | 1:B:777:ASN:HB3   | 1.50                     | 0.77              |
| 1:B:330:THR:O     | 1:B:362:ARG:HD3   | 1.84                     | 0.77              |
| 1:B:697:PHE:CE1   | 1:B:1042:MET:HE2  | 2.20                     | 0.77              |
| 1:A:739:GLN:HE22  | 1:A:777:ASN:HB3   | 1.49                     | 0.76              |
| 1:A:697:PHE:CE1   | 1:A:1042:MET:HE2  | 2.20                     | 0.76              |
| 5:B:1243:TPP:H7'2 | 6:B:1246:PYR:O    | 1.86                     | 0.76              |
| 1:A:1193:GLU:OE1  | 1:B:1077:ARG:HA   | 1.86                     | 0.76              |
| 1:B:1137:LEU:HD22 | 1:B:1141:PHE:HB2  | 1.67                     | 0.76              |
| 1:A:639:PHE:CE2   | 1:A:672:PHE:HB2   | 2.22                     | 0.75              |
| 1:A:1137:LEU:HD22 | 1:A:1141:PHE:HB2  | 1.67                     | 0.75              |
| 5:A:1236:TPP:H7'2 | 6:A:1239:PYR:O    | 1.86                     | 0.75              |
| 1:B:110:HIS:HD2   | 1:B:169:HIS:HD2   | 1.36                     | 0.74              |
| 1:B:639:PHE:CE2   | 1:B:672:PHE:HB2   | 2.22                     | 0.74              |
| 1:A:857:ARG:HG3   | 1:A:858:LEU:HD13  | 1.69                     | 0.74              |
| 1:A:24:VAL:HG13   | 1:B:881:MET:HE2   | 1.69                     | 0.74              |
| 1:B:857:ARG:HG3   | 1:B:858:LEU:HD13  | 1.69                     | 0.74              |
| 1:A:110:HIS:HD2   | 1:A:169:HIS:HD2   | 1.36                     | 0.74              |
| 1:A:1201:PRO:HG3  | 1:B:455:TYR:HB2   | 1.69                     | 0.73              |
| 1:A:234:PRO:HA    | 1:A:237:LEU:HD12  | 1.71                     | 0.73              |
| 1:A:1200:THR:HG23 | 1:A:1202:MET:HE3  | 1.72                     | 0.72              |
| 1:B:234:PRO:HA    | 1:B:237:LEU:HD12  | 1.71                     | 0.72              |
| 1:B:523:ASP:HA    | 1:B:531:LYS:NZ    | 2.05                     | 0.72              |
| 1:B:1200:THR:HG23 | 1:B:1202:MET:HE3  | 1.72                     | 0.72              |
| 1:B:14:THR:HG22   | 1:B:149:ALA:HB1   | 1.72                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:14:THR:HG22   | 1:A:149:ALA:HB1   | 1.72                     | 0.72              |
| 1:A:523:ASP:HA    | 1:A:531:LYS:NZ    | 2.05                     | 0.72              |
| 1:B:126:ASP:HA    | 1:B:329:ARG:HD3   | 1.71                     | 0.71              |
| 1:A:126:ASP:HA    | 1:A:329:ARG:HD3   | 1.71                     | 0.71              |
| 1:A:523:ASP:HA    | 1:A:531:LYS:HZ3   | 1.56                     | 0.70              |
| 1:B:561:MET:HE1   | 1:B:583:LEU:HD21  | 1.71                     | 0.70              |
| 1:A:561:MET:HE1   | 1:A:583:LEU:HD21  | 1.71                     | 0.70              |
| 1:B:180:ILE:HD11  | 1:B:438:ILE:HG21  | 1.72                     | 0.70              |
| 1:A:130:ILE:HG13  | 1:A:131:TYR:H     | 1.56                     | 0.70              |
| 1:B:82:THR:HG22   | 1:B:83:THR:H      | 1.57                     | 0.69              |
| 1:A:180:ILE:HD11  | 1:A:438:ILE:HG21  | 1.72                     | 0.69              |
| 1:A:467:HIS:HB3   | 1:A:481:VAL:HG23  | 1.75                     | 0.69              |
| 1:A:873:ALA:HA    | 1:A:959:ILE:HD13  | 1.75                     | 0.68              |
| 1:B:130:ILE:HG13  | 1:B:131:TYR:H     | 1.56                     | 0.68              |
| 1:A:697:PHE:HD2   | 1:A:800:GLN:NE2   | 1.92                     | 0.68              |
| 1:B:467:HIS:HB3   | 1:B:481:VAL:HG23  | 1.75                     | 0.68              |
| 1:B:643:VAL:O     | 1:B:647:LEU:HG    | 1.94                     | 0.68              |
| 1:A:82:THR:HG22   | 1:A:83:THR:H      | 1.57                     | 0.67              |
| 1:A:643:VAL:O     | 1:A:647:LEU:HG    | 1.94                     | 0.67              |
| 1:B:883:MET:O     | 1:B:887:ARG:HB2   | 1.95                     | 0.67              |
| 1:B:1129:MET:HE3  | 1:B:1149:ARG:NE   | 2.09                     | 0.67              |
| 1:A:883:MET:O     | 1:A:887:ARG:HB2   | 1.95                     | 0.67              |
| 1:A:1129:MET:HE3  | 1:A:1149:ARG:NE   | 2.09                     | 0.67              |
| 1:B:873:ALA:HA    | 1:B:959:ILE:HD13  | 1.75                     | 0.67              |
| 1:B:697:PHE:HD2   | 1:B:800:GLN:NE2   | 1.92                     | 0.66              |
| 1:A:1181:LYS:H    | 1:B:1019:ARG:HH12 | 1.43                     | 0.66              |
| 1:A:460:SER:HB3   | 1:A:746:MET:HE2   | 1.77                     | 0.66              |
| 1:A:1166:MET:O    | 1:A:1169:THR:HG22 | 1.96                     | 0.66              |
| 1:A:141:LEU:HD13  | 1:A:152:MET:HG3   | 1.77                     | 0.66              |
| 1:B:1077:ARG:HH11 | 1:B:1077:ARG:HB2  | 1.61                     | 0.66              |
| 1:B:771:ARG:O     | 1:B:775:VAL:HG23  | 1.96                     | 0.66              |
| 1:B:460:SER:HB3   | 1:B:746:MET:HE2   | 1.77                     | 0.65              |
| 1:A:771:ARG:O     | 1:A:775:VAL:HG23  | 1.96                     | 0.65              |
| 1:B:1035:VAL:HG22 | 1:B:1062:PRO:HB2  | 1.79                     | 0.65              |
| 1:B:1166:MET:O    | 1:B:1169:THR:HG22 | 1.96                     | 0.65              |
| 1:A:456:ASP:HB2   | 1:A:463:ILE:O     | 1.96                     | 0.65              |
| 1:A:881:MET:HE2   | 1:B:24:VAL:HG13   | 1.79                     | 0.65              |
| 1:B:141:LEU:HD13  | 1:B:152:MET:HG3   | 1.77                     | 0.65              |
| 1:A:1077:ARG:HH11 | 1:A:1077:ARG:HB2  | 1.61                     | 0.64              |
| 1:A:154:LEU:HD22  | 1:A:158:LEU:HD11  | 1.79                     | 0.64              |
| 1:B:456:ASP:HB2   | 1:B:463:ILE:O     | 1.96                     | 0.64              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:667:LEU:HB3   | 1:A:853:TYR:O    | 1.97                     | 0.64              |
| 1:B:154:LEU:HD22  | 1:B:158:LEU:HD11 | 1.80                     | 0.64              |
| 1:A:1035:VAL:HG22 | 1:A:1062:PRO:HB2 | 1.79                     | 0.64              |
| 1:B:667:LEU:HB3   | 1:B:853:TYR:O    | 1.97                     | 0.64              |
| 1:B:697:PHE:HE1   | 1:B:1042:MET:HE2 | 1.62                     | 0.64              |
| 1:A:368:LYS:NZ    | 1:B:227:GLN:HE22 | 1.95                     | 0.64              |
| 1:A:1216:ARG:HA   | 1:B:746:MET:O    | 1.97                     | 0.64              |
| 1:B:968:ASP:OD1   | 1:B:1003:LYS:HB2 | 1.99                     | 0.63              |
| 1:A:1232:LYS:NZ   | 1:A:1232:LYS:HB3 | 2.14                     | 0.63              |
| 1:A:730:GLU:CD    | 1:A:730:GLU:H    | 2.05                     | 0.63              |
| 1:A:779:GLU:HB3   | 1:A:783:ARG:NH1  | 2.13                     | 0.63              |
| 1:B:64:GLU:HG3    | 1:B:89:GLY:HA2   | 1.81                     | 0.63              |
| 1:B:730:GLU:H     | 1:B:730:GLU:CD   | 2.05                     | 0.63              |
| 1:B:1193:GLU:N    | 1:B:1193:GLU:CD  | 2.57                     | 0.63              |
| 1:B:523:ASP:HA    | 1:B:531:LYS:HZ3  | 1.63                     | 0.63              |
| 1:B:779:GLU:HB3   | 1:B:783:ARG:NH1  | 2.13                     | 0.63              |
| 1:A:64:GLU:HG3    | 1:A:89:GLY:HA2   | 1.81                     | 0.63              |
| 1:B:445:THR:HG21  | 1:B:574:LEU:HD21 | 1.80                     | 0.63              |
| 1:B:1200:THR:CG2  | 1:B:1202:MET:HE3 | 2.29                     | 0.63              |
| 1:A:34:SER:O      | 1:A:38:GLU:HG3   | 1.98                     | 0.63              |
| 1:A:917:LYS:HB3   | 1:A:917:LYS:HZ3  | 1.64                     | 0.63              |
| 1:B:34:SER:O      | 1:B:38:GLU:HG3   | 1.97                     | 0.63              |
| 1:A:445:THR:HG21  | 1:A:574:LEU:HD21 | 1.80                     | 0.62              |
| 1:B:438:ILE:HG23  | 1:B:449:ALA:HB1  | 1.80                     | 0.62              |
| 1:B:890:LEU:HD11  | 1:B:945:ILE:HG23 | 1.81                     | 0.62              |
| 1:A:1193:GLU:CD   | 1:A:1193:GLU:N   | 2.57                     | 0.62              |
| 1:B:1198:ASP:OD1  | 1:B:1200:THR:HB  | 2.00                     | 0.62              |
| 1:A:890:LEU:HD11  | 1:A:945:ILE:HG23 | 1.81                     | 0.62              |
| 1:A:968:ASP:OD1   | 1:A:1003:LYS:HB2 | 1.99                     | 0.62              |
| 1:A:438:ILE:HG23  | 1:A:449:ALA:HB1  | 1.80                     | 0.62              |
| 1:A:1141:PHE:HZ   | 1:B:1184:GLY:CA  | 2.10                     | 0.62              |
| 1:B:1232:LYS:NZ   | 1:B:1232:LYS:HB3 | 2.14                     | 0.62              |
| 1:A:142:ALA:HB2   | 1:A:170:PHE:CZ   | 2.35                     | 0.62              |
| 1:A:325:THR:CG2   | 1:A:382:MET:SD   | 2.88                     | 0.62              |
| 1:B:522:MET:SD    | 1:B:526:LEU:HD13 | 2.40                     | 0.62              |
| 1:A:1200:THR:CG2  | 1:A:1202:MET:HE3 | 2.29                     | 0.62              |
| 1:B:142:ALA:HB2   | 1:B:170:PHE:CZ   | 2.35                     | 0.62              |
| 1:A:1198:ASP:OD1  | 1:A:1200:THR:HB  | 1.99                     | 0.62              |
| 1:B:467:HIS:CD2   | 1:B:481:VAL:H    | 2.18                     | 0.61              |
| 1:A:325:THR:HG23  | 1:A:382:MET:SD   | 2.40                     | 0.61              |
| 1:B:325:THR:CG2   | 1:B:382:MET:SD   | 2.88                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:467:HIS:CD2  | 1:A:481:VAL:H     | 2.18                     | 0.61              |
| 1:B:148:GLU:O    | 1:B:152:MET:HB2   | 2.00                     | 0.61              |
| 1:A:148:GLU:O    | 1:A:152:MET:HB2   | 2.00                     | 0.61              |
| 1:B:325:THR:HG23 | 1:B:382:MET:SD    | 2.41                     | 0.61              |
| 1:B:1124:VAL:O   | 1:B:1127:PHE:HB3  | 2.01                     | 0.61              |
| 1:A:398:VAL:HG13 | 1:A:656:VAL:CG2   | 2.31                     | 0.61              |
| 1:A:180:ILE:HD11 | 1:A:438:ILE:CG2   | 2.30                     | 0.61              |
| 1:A:522:MET:SD   | 1:A:526:LEU:HD13  | 2.40                     | 0.61              |
| 1:A:1124:VAL:O   | 1:A:1127:PHE:HB3  | 2.01                     | 0.61              |
| 1:B:180:ILE:HD11 | 1:B:438:ILE:CG2   | 2.30                     | 0.60              |
| 1:B:398:VAL:HG13 | 1:B:656:VAL:CG2   | 2.31                     | 0.60              |
| 1:A:993:VAL:HG22 | 1:A:1000:GLN:O    | 2.01                     | 0.60              |
| 1:A:697:PHE:HE1  | 1:A:1042:MET:HE2  | 1.62                     | 0.60              |
| 1:A:154:LEU:HD22 | 1:A:158:LEU:CD1   | 2.31                     | 0.60              |
| 1:A:465:ILE:HD12 | 1:A:466:SER:N     | 2.17                     | 0.60              |
| 1:B:1129:MET:HE3 | 1:B:1149:ARG:CZ   | 2.31                     | 0.60              |
| 1:B:993:VAL:HG22 | 1:B:1000:GLN:O    | 2.01                     | 0.60              |
| 1:B:917:LYS:HZ3  | 1:B:917:LYS:HB3   | 1.66                     | 0.59              |
| 1:B:779:GLU:HB3  | 1:B:783:ARG:HH12  | 1.68                     | 0.59              |
| 1:A:976:HIS:CD2  | 1:B:1003:LYS:HD3  | 2.38                     | 0.59              |
| 1:A:1129:MET:HE3 | 1:A:1149:ARG:CZ   | 2.32                     | 0.59              |
| 1:B:1193:GLU:CD  | 1:B:1193:GLU:H    | 2.11                     | 0.59              |
| 1:B:154:LEU:HD22 | 1:B:158:LEU:CD1   | 2.31                     | 0.59              |
| 1:A:236:TYR:HA   | 1:A:239:VAL:HG12  | 1.84                     | 0.59              |
| 1:B:465:ILE:HD12 | 1:B:466:SER:N     | 2.17                     | 0.59              |
| 1:A:700:PRO:HG3  | 1:A:814:GLY:HA2   | 1.85                     | 0.59              |
| 1:A:1016:ALA:HB1 | 1:A:1019:ARG:HH21 | 1.66                     | 0.59              |
| 1:A:549:ILE:O    | 1:A:553:VAL:HG22  | 2.03                     | 0.59              |
| 1:B:700:PRO:HG3  | 1:B:814:GLY:HA2   | 1.85                     | 0.59              |
| 1:A:356:PRO:O    | 1:A:357:LYS:HB3   | 2.02                     | 0.59              |
| 1:A:1181:LYS:H   | 1:B:1019:ARG:NH1  | 2.01                     | 0.59              |
| 1:B:549:ILE:O    | 1:B:553:VAL:HG22  | 2.03                     | 0.59              |
| 1:B:639:PHE:CD2  | 1:B:672:PHE:HB2   | 2.37                     | 0.59              |
| 1:B:894:ALA:CB   | 1:B:914:LEU:HD21  | 2.33                     | 0.59              |
| 1:B:917:LYS:HB3  | 1:B:917:LYS:NZ    | 2.18                     | 0.59              |
| 1:A:87:SER:HA    | 1:A:129:ASP:HB3   | 1.85                     | 0.59              |
| 1:A:639:PHE:CD2  | 1:A:672:PHE:HB2   | 2.37                     | 0.59              |
| 1:A:676:GLY:HA3  | 1:A:743:LEU:HD22  | 1.84                     | 0.59              |
| 1:A:917:LYS:HB3  | 1:A:917:LYS:NZ    | 2.18                     | 0.59              |
| 1:A:494:TYR:HB3  | 1:A:500:ILE:HD11  | 1.84                     | 0.59              |
| 1:A:894:ALA:CB   | 1:A:914:LEU:HD21  | 2.33                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1048:GLN:HE21 | 1:A:1048:GLN:C    | 2.11                     | 0.58              |
| 1:A:1077:ARG:HA   | 1:B:1193:GLU:OE1  | 2.02                     | 0.58              |
| 1:B:494:TYR:HB3   | 1:B:500:ILE:HD11  | 1.84                     | 0.58              |
| 1:A:396:ASP:HA    | 1:A:656:VAL:HG13  | 1.84                     | 0.58              |
| 1:A:832:MET:HE2   | 1:A:834:ILE:CD1   | 2.31                     | 0.58              |
| 1:B:87:SER:HA     | 1:B:129:ASP:HB3   | 1.85                     | 0.58              |
| 1:B:643:VAL:HB    | 1:B:849:PRO:HB2   | 1.85                     | 0.58              |
| 1:B:676:GLY:HA3   | 1:B:743:LEU:HD22  | 1.84                     | 0.58              |
| 1:A:9:ASP:HA      | 1:A:179:GLU:O     | 2.03                     | 0.58              |
| 1:A:460:SER:HB3   | 1:A:746:MET:CE    | 2.33                     | 0.58              |
| 1:A:643:VAL:HB    | 1:A:849:PRO:HB2   | 1.85                     | 0.58              |
| 1:B:894:ALA:HB3   | 1:B:914:LEU:HD21  | 1.86                     | 0.58              |
| 1:B:1016:ALA:HB1  | 1:B:1019:ARG:HH21 | 1.66                     | 0.58              |
| 1:A:263:TYR:CZ    | 1:A:318:PRO:HG2   | 2.38                     | 0.58              |
| 1:A:699:CYS:SG    | 1:A:703:ALA:HB3   | 2.44                     | 0.58              |
| 1:A:1193:GLU:CD   | 1:A:1193:GLU:H    | 2.11                     | 0.58              |
| 1:B:396:ASP:HA    | 1:B:656:VAL:HG13  | 1.84                     | 0.58              |
| 1:B:806:MET:SD    | 1:B:852:PRO:HB2   | 2.44                     | 0.58              |
| 1:B:1048:GLN:C    | 1:B:1048:GLN:HE21 | 2.11                     | 0.58              |
| 1:A:779:GLU:HB3   | 1:A:783:ARG:HH12  | 1.68                     | 0.58              |
| 1:A:894:ALA:HB3   | 1:A:914:LEU:HD21  | 1.86                     | 0.58              |
| 1:B:699:CYS:SG    | 1:B:703:ALA:HB3   | 2.44                     | 0.58              |
| 1:B:10:GLY:O      | 1:B:14:THR:HG23   | 2.04                     | 0.58              |
| 1:A:806:MET:SD    | 1:A:852:PRO:HB2   | 2.44                     | 0.58              |
| 1:A:1160:PHE:O    | 1:A:1164:GLU:HG3  | 2.04                     | 0.57              |
| 1:B:4:LYS:HB3     | 1:B:185:VAL:HG23  | 1.86                     | 0.57              |
| 1:B:236:TYR:HA    | 1:B:239:VAL:HG12  | 1.84                     | 0.57              |
| 1:A:10:GLY:O      | 1:A:14:THR:HG23   | 2.04                     | 0.57              |
| 1:B:460:SER:HB3   | 1:B:746:MET:CE    | 2.33                     | 0.57              |
| 1:B:9:ASP:HA      | 1:B:179:GLU:O     | 2.03                     | 0.57              |
| 1:B:356:PRO:O     | 1:B:357:LYS:HB3   | 2.02                     | 0.57              |
| 1:B:1160:PHE:O    | 1:B:1164:GLU:HG3  | 2.04                     | 0.57              |
| 1:A:4:LYS:HB3     | 1:A:185:VAL:HG23  | 1.86                     | 0.57              |
| 1:B:20:ALA:HB2    | 1:B:188:TYR:CE1   | 2.39                     | 0.57              |
| 1:B:263:TYR:CZ    | 1:B:318:PRO:HG2   | 2.38                     | 0.57              |
| 1:A:20:ALA:HB2    | 1:A:188:TYR:CE1   | 2.39                     | 0.57              |
| 1:A:565:THR:HG21  | 1:A:609:ALA:HB3   | 1.87                     | 0.57              |
| 1:A:1219:THR:CG2  | 1:A:1221:GLU:HG2  | 2.35                     | 0.57              |
| 5:B:1243:TPP:H2   | 5:B:1243:TPP:HN42 | 1.70                     | 0.57              |
| 1:B:495:VAL:HG23  | 1:B:530:ILE:HD12  | 1.87                     | 0.57              |
| 1:A:697:PHE:CD2   | 1:A:800:GLN:NE2   | 2.73                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1102:ASP:CG   | 1:A:1104:ARG:HH11 | 2.14                     | 0.56              |
| 1:B:1219:THR:CG2  | 1:B:1221:GLU:HG2  | 2.35                     | 0.56              |
| 1:A:1219:THR:HG21 | 1:B:1082:LYS:HZ3  | 1.70                     | 0.56              |
| 1:A:110:HIS:HD2   | 1:A:169:HIS:CD2   | 2.22                     | 0.56              |
| 1:A:986:VAL:HG22  | 1:A:1064:LEU:HD23 | 1.88                     | 0.56              |
| 1:B:345:CYS:O     | 1:B:349:VAL:HG13  | 2.06                     | 0.56              |
| 1:A:1215:ASN:ND2  | 1:B:1080:MET:H    | 2.03                     | 0.56              |
| 1:B:467:HIS:HD2   | 1:B:481:VAL:H     | 1.53                     | 0.56              |
| 1:B:697:PHE:CD2   | 1:B:800:GLN:NE2   | 2.73                     | 0.56              |
| 1:B:986:VAL:HG22  | 1:B:1064:LEU:HD23 | 1.88                     | 0.56              |
| 1:B:1225:ASP:O    | 1:B:1229:ARG:HG3  | 2.06                     | 0.56              |
| 1:B:434:ASN:O     | 1:B:438:ILE:HG13  | 2.06                     | 0.56              |
| 1:B:565:THR:HG21  | 1:B:609:ALA:HB3   | 1.87                     | 0.56              |
| 1:B:832:MET:HE2   | 1:B:834:ILE:CD1   | 2.31                     | 0.56              |
| 1:A:20:ALA:HB2    | 1:A:188:TYR:CZ    | 2.40                     | 0.56              |
| 1:B:124:PHE:CB    | 1:B:367:SER:HB2   | 2.26                     | 0.55              |
| 1:B:1004:ALA:O    | 1:B:1022:LYS:HG3  | 2.06                     | 0.55              |
| 1:B:1102:ASP:CG   | 1:B:1104:ARG:HH11 | 2.14                     | 0.55              |
| 5:A:1236:TPP:H2   | 5:A:1236:TPP:HN42 | 1.70                     | 0.55              |
| 1:B:290:LEU:HG    | 1:B:295:GLU:OE1   | 2.07                     | 0.55              |
| 1:A:1004:ALA:O    | 1:A:1022:LYS:HG3  | 2.06                     | 0.55              |
| 1:A:1225:ASP:O    | 1:A:1229:ARG:HG3  | 2.06                     | 0.55              |
| 1:B:20:ALA:HB2    | 1:B:188:TYR:CZ    | 2.40                     | 0.55              |
| 1:A:345:CYS:O     | 1:A:349:VAL:HG13  | 2.06                     | 0.55              |
| 1:B:681:VAL:HG23  | 1:B:770:GLN:HG3   | 1.88                     | 0.55              |
| 1:B:715:VAL:C     | 1:B:717:ALA:H     | 2.14                     | 0.55              |
| 1:A:561:MET:HE1   | 1:A:583:LEU:CD2   | 2.36                     | 0.55              |
| 1:A:495:VAL:HG23  | 1:A:530:ILE:HD12  | 1.87                     | 0.55              |
| 1:A:563:MET:HE3   | 1:A:563:MET:HA    | 1.89                     | 0.55              |
| 1:B:260:LEU:O     | 1:B:303:ARG:HB2   | 2.07                     | 0.55              |
| 1:B:1232:LYS:HB3  | 1:B:1232:LYS:HZ2  | 1.72                     | 0.55              |
| 5:B:1243:TPP:H7'2 | 6:B:1246:PYR:C    | 2.36                     | 0.55              |
| 1:A:536:ASN:HD22  | 1:A:623:LYS:NZ    | 2.05                     | 0.55              |
| 5:A:1236:TPP:H7'2 | 6:A:1239:PYR:C    | 2.36                     | 0.55              |
| 1:B:331:LYS:HG3   | 1:B:331:LYS:O     | 2.06                     | 0.55              |
| 1:A:681:VAL:HG23  | 1:A:770:GLN:HG3   | 1.88                     | 0.55              |
| 1:B:1219:THR:HG22 | 1:B:1222:GLN:H    | 1.72                     | 0.55              |
| 1:A:434:ASN:O     | 1:A:438:ILE:HG13  | 2.06                     | 0.55              |
| 1:B:495:VAL:HG13  | 1:B:496:GLY:N     | 2.22                     | 0.55              |
| 1:A:456:ASP:OD1   | 1:A:458:LYS:HB2   | 2.07                     | 0.55              |
| 1:B:110:HIS:CD2   | 1:B:169:HIS:CD2   | 2.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1077:ARG:HB2  | 1:B:1077:ARG:NH1  | 2.22                     | 0.55              |
| 1:B:422:PHE:HE1   | 1:B:468:LEU:HG    | 1.72                     | 0.54              |
| 1:A:422:PHE:HE1   | 1:A:468:LEU:HG    | 1.72                     | 0.54              |
| 1:A:495:VAL:HG13  | 1:A:496:GLY:N     | 2.22                     | 0.54              |
| 1:A:715:VAL:C     | 1:A:717:ALA:H     | 2.13                     | 0.54              |
| 1:B:563:MET:HE3   | 1:B:563:MET:HA    | 1.89                     | 0.54              |
| 1:A:1219:THR:HG22 | 1:A:1222:GLN:H    | 1.72                     | 0.54              |
| 1:B:58:ILE:HD12   | 1:B:58:ILE:H      | 1.72                     | 0.54              |
| 1:B:456:ASP:OD1   | 1:B:458:LYS:HB2   | 2.07                     | 0.54              |
| 1:B:561:MET:HE1   | 1:B:583:LEU:CD2   | 2.36                     | 0.54              |
| 1:B:1146:LYS:HA   | 1:B:1149:ARG:HH12 | 1.72                     | 0.54              |
| 1:A:495:VAL:HG13  | 1:A:496:GLY:H     | 1.73                     | 0.54              |
| 1:A:260:LEU:O     | 1:A:303:ARG:HB2   | 2.07                     | 0.54              |
| 1:A:434:ASN:HD22  | 1:A:453:PHE:HE1   | 1.56                     | 0.54              |
| 1:A:467:HIS:HD2   | 1:A:481:VAL:H     | 1.54                     | 0.54              |
| 1:A:99:LYS:HE3    | 1:B:867:SER:O     | 2.06                     | 0.54              |
| 1:A:249:LYS:O     | 1:A:252:SER:HB3   | 2.07                     | 0.54              |
| 1:A:1146:LYS:HA   | 1:A:1149:ARG:HH12 | 1.72                     | 0.54              |
| 1:B:323:VAL:CG1   | 1:B:382:MET:HG2   | 2.38                     | 0.54              |
| 1:B:688:ASN:HD21  | 1:B:759:GLU:HB2   | 1.73                     | 0.54              |
| 1:B:1149:ARG:HH11 | 1:B:1149:ARG:CG   | 2.16                     | 0.54              |
| 1:A:64:GLU:HB2    | 1:A:93:MET:HE3    | 1.89                     | 0.54              |
| 1:A:210:PRO:HB2   | 1:B:831:ARG:HA    | 1.89                     | 0.54              |
| 1:A:290:LEU:HG    | 1:A:295:GLU:OE1   | 2.07                     | 0.54              |
| 1:A:1131:GLN:OE1  | 1:A:1133:ARG:NE   | 2.40                     | 0.54              |
| 1:A:497:ILE:HG13  | 1:A:498:TYR:CD2   | 2.43                     | 0.53              |
| 1:B:536:ASN:HD22  | 1:B:623:LYS:NZ    | 2.05                     | 0.53              |
| 1:B:817:GLU:HB3   | 1:B:989:MET:HE3   | 1.90                     | 0.53              |
| 1:A:227:GLN:HE22  | 1:B:368:LYS:NZ    | 2.07                     | 0.53              |
| 1:A:609:ALA:O     | 1:A:613:LEU:HB2   | 2.08                     | 0.53              |
| 1:B:249:LYS:O     | 1:B:252:SER:HB3   | 2.07                     | 0.53              |
| 1:B:1230:THR:O    | 1:B:1232:LYS:N    | 2.42                     | 0.53              |
| 1:A:323:VAL:CG1   | 1:A:382:MET:HG2   | 2.38                     | 0.53              |
| 1:A:688:ASN:HD21  | 1:A:759:GLU:HB2   | 1.73                     | 0.53              |
| 1:A:1194:PHE:CD2  | 1:A:1213:ASP:HB3  | 2.44                     | 0.53              |
| 1:B:495:VAL:HG13  | 1:B:496:GLY:H     | 1.73                     | 0.53              |
| 1:A:1219:THR:HG21 | 1:B:1082:LYS:NZ   | 2.24                     | 0.53              |
| 1:A:331:LYS:O     | 1:A:331:LYS:HG3   | 2.06                     | 0.53              |
| 1:A:536:ASN:HD22  | 1:A:623:LYS:HZ3   | 1.57                     | 0.53              |
| 1:A:699:CYS:HA    | 4:A:1234:SF4:S2   | 2.48                     | 0.53              |
| 1:A:1080:MET:O    | 1:A:1083:SER:HB2  | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1080:MET:O    | 1:B:1083:SER:HB2  | 2.08                     | 0.53              |
| 1:A:110:HIS:CD2   | 1:A:169:HIS:CD2   | 2.88                     | 0.53              |
| 1:A:817:GLU:HB3   | 1:A:989:MET:HE3   | 1.91                     | 0.53              |
| 1:B:609:ALA:O     | 1:B:613:LEU:HB2   | 2.08                     | 0.53              |
| 1:A:463:ILE:HG13  | 1:A:464:THR:N     | 2.24                     | 0.53              |
| 1:A:903:SER:O     | 1:A:907:LYS:HG3   | 2.08                     | 0.53              |
| 1:B:64:GLU:HB2    | 1:B:93:MET:HE3    | 1.89                     | 0.53              |
| 1:B:221:ASN:HB3   | 1:B:222:PRO:CD    | 2.39                     | 0.53              |
| 1:B:867:SER:O     | 1:B:868:LEU:HD23  | 2.09                     | 0.53              |
| 1:B:903:SER:O     | 1:B:907:LYS:HG3   | 2.08                     | 0.53              |
| 1:B:1131:GLN:OE1  | 1:B:1133:ARG:NE   | 2.40                     | 0.53              |
| 1:A:1077:ARG:HB2  | 1:A:1077:ARG:NH1  | 2.22                     | 0.53              |
| 1:B:630:LYS:HD2   | 1:B:632:GLU:HG2   | 1.91                     | 0.53              |
| 1:B:1194:PHE:CD2  | 1:B:1213:ASP:HB3  | 2.44                     | 0.53              |
| 1:A:630:LYS:HD2   | 1:A:632:GLU:HG2   | 1.91                     | 0.53              |
| 1:A:1149:ARG:HH11 | 1:A:1149:ARG:CG   | 2.16                     | 0.53              |
| 1:A:398:VAL:HG13  | 1:A:656:VAL:HG22  | 1.91                     | 0.52              |
| 1:A:1059:PHE:HD1  | 1:A:1104:ARG:HD3  | 1.75                     | 0.52              |
| 1:A:1082:LYS:HZ3  | 1:B:1219:THR:HG21 | 1.74                     | 0.52              |
| 1:B:534:ILE:HA    | 1:B:539:LEU:HG    | 1.91                     | 0.52              |
| 1:B:619:PRO:HG2   | 1:B:622:TRP:CD1   | 2.44                     | 0.52              |
| 1:A:867:SER:O     | 1:A:868:LEU:HD23  | 2.09                     | 0.52              |
| 1:A:1230:THR:O    | 1:A:1232:LYS:N    | 2.42                     | 0.52              |
| 1:B:497:ILE:HG13  | 1:B:498:TYR:CD2   | 2.43                     | 0.52              |
| 1:B:699:CYS:HA    | 4:B:1241:SF4:S2   | 2.48                     | 0.52              |
| 1:A:81:THR:HG22   | 1:A:82:THR:N      | 2.24                     | 0.52              |
| 1:A:387:LYS:HD3   | 1:A:390:PHE:HB3   | 1.91                     | 0.52              |
| 1:A:1019:ARG:HH12 | 1:B:1181:LYS:H    | 1.57                     | 0.52              |
| 1:B:434:ASN:HD22  | 1:B:453:PHE:HE1   | 1.56                     | 0.52              |
| 1:A:964:GLY:O     | 1:A:968:ASP:HB2   | 2.10                     | 0.52              |
| 1:A:323:VAL:HA    | 1:A:356:PRO:O     | 2.09                     | 0.52              |
| 1:B:387:LYS:HD3   | 1:B:390:PHE:HB3   | 1.91                     | 0.52              |
| 1:B:775:VAL:HB    | 1:B:776:PRO:CD    | 2.40                     | 0.52              |
| 1:B:964:GLY:O     | 1:B:968:ASP:HB2   | 2.10                     | 0.52              |
| 1:A:775:VAL:HB    | 1:A:776:PRO:CD    | 2.40                     | 0.52              |
| 1:B:398:VAL:HG13  | 1:B:656:VAL:HG22  | 1.91                     | 0.52              |
| 1:A:58:ILE:HD12   | 1:A:58:ILE:H      | 1.72                     | 0.52              |
| 1:B:463:ILE:HG13  | 1:B:464:THR:N     | 2.24                     | 0.52              |
| 1:B:1059:PHE:HD1  | 1:B:1104:ARG:HD3  | 1.75                     | 0.52              |
| 1:A:230:GLU:OE2   | 1:B:331:LYS:HE3   | 2.09                     | 0.52              |
| 1:A:534:ILE:HA    | 1:A:539:LEU:HG    | 1.91                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:1036:TYR:O   | 1:B:1063:SER:HA   | 2.10                     | 0.52              |
| 1:A:619:PRO:HG2  | 1:A:622:TRP:CD1   | 2.44                     | 0.52              |
| 1:A:853:TYR:CE2  | 1:A:864:TRP:CD1   | 2.98                     | 0.52              |
| 1:A:1035:VAL:O   | 1:A:1037:VAL:HG23 | 2.10                     | 0.52              |
| 1:B:323:VAL:HA   | 1:B:356:PRO:O     | 2.09                     | 0.52              |
| 1:A:221:ASN:HB3  | 1:A:222:PRO:CD    | 2.39                     | 0.51              |
| 1:A:681:VAL:HG22 | 1:A:767:LEU:HA    | 1.91                     | 0.51              |
| 1:B:81:THR:HG22  | 1:B:82:THR:N      | 2.24                     | 0.51              |
| 1:A:269:ALA:HA   | 1:A:296:LYS:HB3   | 1.92                     | 0.51              |
| 1:A:873:ALA:HA   | 1:A:959:ILE:HG21  | 1.92                     | 0.51              |
| 1:A:961:GLY:O    | 1:A:988:VAL:HA    | 2.11                     | 0.51              |
| 1:A:1025:LEU:O   | 1:A:1029:VAL:HG13 | 2.11                     | 0.51              |
| 1:A:1036:TYR:O   | 1:A:1063:SER:HA   | 2.10                     | 0.51              |
| 1:B:873:ALA:HA   | 1:B:959:ILE:HG21  | 1.92                     | 0.51              |
| 1:A:105:LEU:O    | 1:A:166:PRO:HG3   | 2.11                     | 0.51              |
| 1:A:695:CYS:HB2  | 1:A:704:ILE:HD13  | 1.92                     | 0.51              |
| 1:B:349:VAL:CG2  | 1:B:350:GLU:N     | 2.73                     | 0.51              |
| 1:B:853:TYR:CE2  | 1:B:864:TRP:CD1   | 2.98                     | 0.51              |
| 1:A:1138:ASP:O   | 1:A:1142:PRO:HG3  | 2.10                     | 0.51              |
| 1:B:465:ILE:HG13 | 1:B:467:HIS:CE1   | 2.46                     | 0.51              |
| 1:A:465:ILE:HG13 | 1:A:467:HIS:CE1   | 2.46                     | 0.51              |
| 1:B:105:LEU:O    | 1:B:166:PRO:HG3   | 2.11                     | 0.51              |
| 1:A:349:VAL:CG2  | 1:A:350:GLU:N     | 2.73                     | 0.51              |
| 1:B:1016:ALA:HB1 | 1:B:1019:ARG:NH2  | 2.26                     | 0.51              |
| 1:B:1035:VAL:O   | 1:B:1037:VAL:HG23 | 2.10                     | 0.51              |
| 1:A:715:VAL:HG12 | 1:A:716:GLY:N     | 2.25                     | 0.51              |
| 1:A:1160:PHE:O   | 1:A:1160:PHE:CD1  | 2.64                     | 0.51              |
| 1:B:681:VAL:HG22 | 1:B:767:LEU:HA    | 1.91                     | 0.51              |
| 1:B:695:CYS:HB2  | 1:B:704:ILE:HD13  | 1.92                     | 0.51              |
| 1:B:1138:ASP:O   | 1:B:1142:PRO:HG3  | 2.10                     | 0.51              |
| 1:B:715:VAL:HG12 | 1:B:716:GLY:N     | 2.25                     | 0.50              |
| 1:B:1160:PHE:O   | 1:B:1160:PHE:CD1  | 2.64                     | 0.50              |
| 1:B:1025:LEU:O   | 1:B:1029:VAL:HG13 | 2.11                     | 0.50              |
| 1:A:130:ILE:HD13 | 1:A:170:PHE:CZ    | 2.46                     | 0.50              |
| 1:A:910:LEU:HD12 | 1:A:930:LEU:HD21  | 1.92                     | 0.50              |
| 1:B:110:HIS:HD2  | 1:B:169:HIS:CD2   | 2.22                     | 0.50              |
| 1:B:131:TYR:O    | 1:B:134:ARG:HB2   | 2.12                     | 0.50              |
| 1:B:902:ALA:O    | 1:B:907:LYS:HE3   | 2.11                     | 0.50              |
| 1:A:491:ASN:C    | 1:A:491:ASN:HD22  | 2.19                     | 0.50              |
| 1:B:691:GLN:HG2  | 1:B:736:PHE:CD1   | 2.47                     | 0.50              |
| 1:B:910:LEU:HD12 | 1:B:930:LEU:HD21  | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:910:LEU:HD13 | 1:B:930:LEU:HD11 | 1.93                     | 0.50              |
| 1:A:869:PHE:CE2  | 1:A:969:ILE:HG21 | 2.47                     | 0.50              |
| 1:B:269:ALA:HA   | 1:B:296:LYS:HB3  | 1.92                     | 0.50              |
| 1:A:82:THR:HG22  | 1:A:83:THR:N     | 2.27                     | 0.50              |
| 1:A:131:TYR:O    | 1:A:134:ARG:HB2  | 2.12                     | 0.50              |
| 1:A:684:TRP:CE2  | 1:A:738:ILE:HB   | 2.47                     | 0.50              |
| 1:A:1016:ALA:HB1 | 1:A:1019:ARG:NH2 | 2.26                     | 0.50              |
| 1:B:578:LYS:HE3  | 1:B:582:LEU:HD21 | 1.94                     | 0.50              |
| 1:A:691:GLN:HG2  | 1:A:736:PHE:CD1  | 2.47                     | 0.50              |
| 1:B:491:ASN:C    | 1:B:491:ASN:HD22 | 2.19                     | 0.50              |
| 1:B:578:LYS:HG3  | 1:B:582:LEU:HD22 | 1.94                     | 0.50              |
| 1:B:587:ILE:O    | 1:B:591:TYR:HB2  | 2.12                     | 0.50              |
| 1:B:869:PHE:CE2  | 1:B:969:ILE:HG21 | 2.46                     | 0.50              |
| 1:B:963:ASP:HB3  | 1:B:990:ASP:OD1  | 2.12                     | 0.50              |
| 1:A:43:TRP:HB3   | 1:A:48:ARG:HD3   | 1.94                     | 0.50              |
| 1:A:216:ARG:O    | 1:B:865:GLY:HA2  | 2.12                     | 0.50              |
| 1:A:578:LYS:HE3  | 1:A:582:LEU:HD21 | 1.94                     | 0.50              |
| 1:A:721:PHE:HD1  | 1:A:777:ASN:HD22 | 1.59                     | 0.50              |
| 1:A:902:ALA:O    | 1:A:907:LYS:HE3  | 2.11                     | 0.50              |
| 1:A:693:ASN:HB3  | 1:A:800:GLN:HB2  | 1.94                     | 0.50              |
| 1:B:961:GLY:O    | 1:B:988:VAL:HA   | 2.11                     | 0.50              |
| 1:B:130:ILE:HD13 | 1:B:170:PHE:CZ   | 2.46                     | 0.49              |
| 1:B:200:LEU:HD11 | 1:B:204:ARG:NH1  | 2.27                     | 0.49              |
| 1:A:200:LEU:HD11 | 1:A:204:ARG:NH1  | 2.27                     | 0.49              |
| 1:A:553:VAL:O    | 1:A:601:MET:HG3  | 2.11                     | 0.49              |
| 1:A:587:ILE:O    | 1:A:591:TYR:HB2  | 2.12                     | 0.49              |
| 1:A:746:MET:O    | 1:B:1216:ARG:HA  | 2.12                     | 0.49              |
| 1:A:910:LEU:HD13 | 1:A:930:LEU:HD11 | 1.93                     | 0.49              |
| 1:B:182:LYS:HE2  | 1:B:442:GLY:O    | 2.13                     | 0.49              |
| 1:A:323:VAL:HG12 | 1:A:382:MET:HG2  | 1.94                     | 0.49              |
| 1:B:512:LEU:HD12 | 1:B:513:ASN:N    | 2.27                     | 0.49              |
| 1:B:636:ASN:ND2  | 1:B:672:PHE:HE2  | 2.11                     | 0.49              |
| 1:A:182:LYS:HE2  | 1:A:442:GLY:O    | 2.13                     | 0.49              |
| 1:A:1188:PHE:HB3 | 1:B:1010:VAL:O   | 2.11                     | 0.49              |
| 1:B:43:TRP:HB3   | 1:B:48:ARG:HD3   | 1.94                     | 0.49              |
| 1:B:721:PHE:HD1  | 1:B:777:ASN:HD22 | 1.59                     | 0.49              |
| 1:B:965:TRP:CE3  | 1:B:966:ALA:HB2  | 2.48                     | 0.49              |
| 1:B:126:ASP:HA   | 1:B:329:ARG:CD   | 2.42                     | 0.49              |
| 1:B:713:GLU:O    | 1:B:780:TYR:OH   | 2.31                     | 0.49              |
| 1:A:691:GLN:HE22 | 1:A:726:ALA:HA   | 1.78                     | 0.49              |
| 1:A:264:VAL:HG21 | 1:A:301:LYS:HE3  | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:883:MET:HE2  | 1:A:955:LYS:HD2  | 1.94                     | 0.49              |
| 1:B:27:ILE:HG23  | 1:B:28:TYR:N     | 2.28                     | 0.49              |
| 1:B:553:VAL:O    | 1:B:601:MET:HG3  | 2.11                     | 0.49              |
| 1:A:334:GLY:O    | 1:B:307:PRO:HA   | 2.13                     | 0.49              |
| 1:A:512:LEU:HD12 | 1:A:513:ASN:N    | 2.28                     | 0.49              |
| 1:B:684:TRP:CE2  | 1:B:738:ILE:HB   | 2.47                     | 0.49              |
| 1:A:965:TRP:CE3  | 1:A:966:ALA:HB2  | 2.48                     | 0.49              |
| 1:B:323:VAL:HG12 | 1:B:382:MET:HG2  | 1.94                     | 0.49              |
| 1:B:883:MET:HE2  | 1:B:955:LYS:HD2  | 1.94                     | 0.49              |
| 1:A:992:GLU:O    | 1:A:993:VAL:HB   | 2.13                     | 0.49              |
| 1:A:578:LYS:HG3  | 1:A:582:LEU:HD22 | 1.94                     | 0.48              |
| 1:A:569:LYS:HB3  | 1:A:570:LEU:HD13 | 1.95                     | 0.48              |
| 1:A:703:ALA:HB3  | 4:A:1234:SF4:S4  | 2.53                     | 0.48              |
| 1:A:994:TYR:CE1  | 1:A:1002:SER:HB2 | 2.48                     | 0.48              |
| 1:B:693:ASN:HB3  | 1:B:800:GLN:HB2  | 1.94                     | 0.48              |
| 1:B:992:GLU:O    | 1:B:993:VAL:HB   | 2.13                     | 0.48              |
| 1:A:27:ILE:HG23  | 1:A:28:TYR:N     | 2.28                     | 0.48              |
| 1:A:681:VAL:CG2  | 1:A:767:LEU:HA   | 2.43                     | 0.48              |
| 1:A:963:ASP:HB3  | 1:A:990:ASP:OD1  | 2.12                     | 0.48              |
| 1:A:1129:MET:HE1 | 1:A:1138:ASP:HB2 | 1.95                     | 0.48              |
| 1:B:23:GLU:OE1   | 1:B:204:ARG:NH2  | 2.46                     | 0.48              |
| 1:B:691:GLN:HE22 | 1:B:726:ALA:HA   | 1.78                     | 0.48              |
| 1:B:703:ALA:HB3  | 4:B:1241:SF4:S4  | 2.53                     | 0.48              |
| 1:A:60:GLU:O     | 1:B:976:HIS:HE1  | 1.96                     | 0.48              |
| 1:A:583:LEU:O    | 1:A:587:ILE:HG12 | 2.13                     | 0.48              |
| 1:A:834:ILE:HD13 | 1:A:960:PHE:CE2  | 2.49                     | 0.48              |
| 1:A:940:GLY:O    | 1:A:943:GLY:N    | 2.46                     | 0.48              |
| 1:B:264:VAL:HG21 | 1:B:301:LYS:HE3  | 1.93                     | 0.48              |
| 1:B:590:ALA:O    | 1:B:591:TYR:HB2  | 2.14                     | 0.48              |
| 1:A:23:GLU:OE1   | 1:A:204:ARG:NH2  | 2.46                     | 0.48              |
| 1:A:274:VAL:HG23 | 1:A:324:ILE:CD1  | 2.44                     | 0.48              |
| 1:A:1019:ARG:NH1 | 1:B:1181:LYS:H   | 2.12                     | 0.48              |
| 1:B:226:PHE:HD1  | 1:B:226:PHE:O    | 1.96                     | 0.48              |
| 1:B:42:ASP:O     | 1:B:46:GLN:HG3   | 2.14                     | 0.48              |
| 1:B:684:TRP:CD2  | 1:B:738:ILE:HB   | 2.48                     | 0.48              |
| 1:A:684:TRP:CD2  | 1:A:738:ILE:HB   | 2.48                     | 0.48              |
| 1:A:42:ASP:O     | 1:A:46:GLN:HG3   | 2.14                     | 0.48              |
| 1:A:338:ASP:OD2  | 1:A:362:ARG:NH1  | 2.47                     | 0.48              |
| 1:A:681:VAL:HG12 | 1:A:745:CYS:SG   | 2.53                     | 0.48              |
| 1:B:274:VAL:HG23 | 1:B:324:ILE:CD1  | 2.44                     | 0.48              |
| 1:B:617:LYS:HB2  | 1:B:617:LYS:NZ   | 2.28                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:721:PHE:CE1  | 1:B:780:TYR:HD2   | 2.32                     | 0.48              |
| 1:B:867:SER:HB2  | 1:B:875:TYR:CG    | 2.49                     | 0.48              |
| 1:B:940:GLY:O    | 1:B:943:GLY:N     | 2.46                     | 0.48              |
| 1:B:994:TYR:CE1  | 1:B:1002:SER:HB2  | 2.48                     | 0.48              |
| 1:A:566:ALA:HA   | 1:A:613:LEU:HD21  | 1.95                     | 0.48              |
| 1:A:867:SER:HB2  | 1:A:875:TYR:CG    | 2.49                     | 0.48              |
| 1:A:590:ALA:O    | 1:A:591:TYR:HB2   | 2.14                     | 0.47              |
| 1:A:713:GLU:O    | 1:A:780:TYR:OH    | 2.31                     | 0.47              |
| 1:A:736:PHE:CD1  | 1:A:736:PHE:C     | 2.92                     | 0.47              |
| 1:B:736:PHE:CD1  | 1:B:736:PHE:C     | 2.92                     | 0.47              |
| 1:B:799:SER:OG   | 1:B:800:GLN:NE2   | 2.47                     | 0.47              |
| 1:A:1175:PHE:CZ  | 1:A:1177:PRO:HA   | 2.49                     | 0.47              |
| 1:B:569:LYS:HB3  | 1:B:570:LEU:HD13  | 1.95                     | 0.47              |
| 1:B:642:VAL:C    | 1:B:645:PRO:HD2   | 2.39                     | 0.47              |
| 1:B:646:ILE:HG21 | 1:B:849:PRO:HD3   | 1.96                     | 0.47              |
| 1:B:681:VAL:CG2  | 1:B:767:LEU:HA    | 2.43                     | 0.47              |
| 1:B:1012:LYS:O   | 1:B:1013:PHE:HB2  | 2.14                     | 0.47              |
| 1:A:154:LEU:HD13 | 1:A:250:VAL:HG22  | 1.96                     | 0.47              |
| 1:A:795:SER:O    | 1:A:796:LEU:C     | 2.58                     | 0.47              |
| 1:B:351:ARG:HD3  | 1:B:353:GLU:HB2   | 1.96                     | 0.47              |
| 1:B:566:ALA:HA   | 1:B:613:LEU:HD21  | 1.95                     | 0.47              |
| 1:B:871:ASP:HB2  | 1:B:874:GLU:HG2   | 1.96                     | 0.47              |
| 1:B:1040:VAL:HA  | 1:B:1098:LEU:HD22 | 1.96                     | 0.47              |
| 1:B:1129:MET:HE1 | 1:B:1138:ASP:HB2  | 1.95                     | 0.47              |
| 1:B:146:VAL:HG12 | 1:B:183:ILE:HD13  | 1.96                     | 0.47              |
| 1:A:636:ASN:ND2  | 1:A:672:PHE:HE2   | 2.11                     | 0.47              |
| 1:A:710:LYS:HD2  | 1:A:734:TYR:HE1   | 1.80                     | 0.47              |
| 1:A:799:SER:OG   | 1:A:800:GLN:NE2   | 2.47                     | 0.47              |
| 1:B:681:VAL:HG12 | 1:B:745:CYS:SG    | 2.53                     | 0.47              |
| 1:B:795:SER:O    | 1:B:796:LEU:C     | 2.58                     | 0.47              |
| 1:A:146:VAL:HG12 | 1:A:183:ILE:HD13  | 1.96                     | 0.47              |
| 1:A:226:PHE:HD1  | 1:A:226:PHE:O     | 1.96                     | 0.47              |
| 1:A:286:VAL:HG12 | 1:A:290:LEU:HD22  | 1.97                     | 0.47              |
| 1:B:121:LEU:HG   | 1:B:122:SER:N     | 2.29                     | 0.47              |
| 1:B:338:ASP:OD2  | 1:B:362:ARG:NH1   | 2.47                     | 0.47              |
| 1:B:536:ASN:HA   | 1:B:623:LYS:HZ3   | 1.79                     | 0.47              |
| 1:B:583:LEU:O    | 1:B:587:ILE:HG12  | 2.13                     | 0.47              |
| 1:B:710:LYS:HD2  | 1:B:734:TYR:HE1   | 1.80                     | 0.47              |
| 1:B:814:GLY:O    | 1:B:1080:MET:HE3  | 2.15                     | 0.47              |
| 1:B:834:ILE:HD13 | 1:B:960:PHE:CE2   | 2.49                     | 0.47              |
| 1:A:617:LYS:HB2  | 1:A:617:LYS:NZ    | 2.28                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1012:LYS:O   | 1:A:1013:PHE:HB2  | 2.14                     | 0.47              |
| 1:A:1214:GLN:NE2 | 1:B:461:GLY:H     | 2.12                     | 0.47              |
| 1:B:573:VAL:HG23 | 1:B:574:LEU:HG    | 1.97                     | 0.47              |
| 1:B:1129:MET:HG2 | 1:B:1149:ARG:HE   | 1.80                     | 0.47              |
| 1:B:1175:PHE:CZ  | 1:B:1177:PRO:HA   | 2.49                     | 0.47              |
| 1:A:121:LEU:HG   | 1:A:122:SER:N     | 2.29                     | 0.47              |
| 1:A:126:ASP:HA   | 1:A:329:ARG:CD    | 2.42                     | 0.47              |
| 1:A:317:LEU:HD22 | 1:A:317:LEU:C     | 2.39                     | 0.47              |
| 1:A:351:ARG:HD3  | 1:A:353:GLU:HB2   | 1.96                     | 0.47              |
| 1:A:779:GLU:C    | 1:A:783:ARG:HH11  | 2.23                     | 0.47              |
| 1:A:867:SER:O    | 1:B:99:LYS:HE3    | 2.15                     | 0.47              |
| 1:A:871:ASP:HB2  | 1:A:874:GLU:HG2   | 1.96                     | 0.47              |
| 1:B:64:GLU:HG3   | 1:B:89:GLY:CA     | 2.45                     | 0.47              |
| 1:B:890:LEU:CD1  | 1:B:945:ILE:HG23  | 2.45                     | 0.47              |
| 1:B:917:LYS:NZ   | 1:B:917:LYS:CB    | 2.78                     | 0.47              |
| 1:A:14:THR:HG21  | 1:A:171:PHE:CE1   | 2.50                     | 0.47              |
| 1:A:573:VAL:HG23 | 1:A:574:LEU:HG    | 1.97                     | 0.47              |
| 1:A:646:ILE:HG21 | 1:A:849:PRO:HD3   | 1.96                     | 0.47              |
| 1:A:1003:LYS:HD3 | 1:B:976:HIS:CD2   | 2.50                     | 0.47              |
| 1:A:721:PHE:CE1  | 1:A:780:TYR:HD2   | 2.32                     | 0.46              |
| 1:A:1214:GLN:CD  | 1:B:461:GLY:H     | 2.23                     | 0.46              |
| 1:B:779:GLU:C    | 1:B:783:ARG:HH11  | 2.23                     | 0.46              |
| 1:B:1007:THR:HB  | 1:B:1152:VAL:HG22 | 1.96                     | 0.46              |
| 1:A:642:VAL:C    | 1:A:645:PRO:HD2   | 2.39                     | 0.46              |
| 1:A:1216:ARG:HE  | 1:B:677:VAL:HG23  | 1.79                     | 0.46              |
| 1:A:1232:LYS:HB3 | 1:A:1232:LYS:HZ2  | 1.79                     | 0.46              |
| 1:B:373:ALA:O    | 1:B:376:LYS:HB3   | 2.15                     | 0.46              |
| 1:B:667:LEU:HD12 | 1:B:667:LEU:N     | 2.31                     | 0.46              |
| 1:B:154:LEU:HD13 | 1:B:250:VAL:HG22  | 1.96                     | 0.46              |
| 1:A:390:PHE:CE2  | 1:A:403:LEU:HD22  | 2.51                     | 0.46              |
| 1:A:667:LEU:N    | 1:A:667:LEU:HD12  | 2.31                     | 0.46              |
| 1:B:694:GLN:O    | 1:B:698:VAL:HB    | 2.16                     | 0.46              |
| 1:A:373:ALA:O    | 1:A:376:LYS:HB3   | 2.15                     | 0.46              |
| 1:A:710:LYS:HD2  | 1:A:734:TYR:CE1   | 2.51                     | 0.46              |
| 1:A:814:GLY:O    | 1:A:1080:MET:HE3  | 2.15                     | 0.46              |
| 1:B:317:LEU:C    | 1:B:317:LEU:HD22  | 2.39                     | 0.46              |
| 1:B:390:PHE:CE2  | 1:B:403:LEU:HD22  | 2.51                     | 0.46              |
| 1:B:693:ASN:HD21 | 1:B:736:PHE:HZ    | 1.63                     | 0.46              |
| 1:B:1200:THR:HA  | 1:B:1201:PRO:HD3  | 1.83                     | 0.46              |
| 1:A:184:GLU:CD   | 1:A:256:ARG:HH12  | 2.23                     | 0.46              |
| 1:A:274:VAL:HG23 | 1:A:324:ILE:HD12  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1048:GLN:C   | 1:A:1048:GLN:NE2  | 2.73                     | 0.46              |
| 1:A:1200:THR:CG2 | 1:A:1202:MET:H    | 2.28                     | 0.46              |
| 1:A:173:GLY:O    | 1:A:174:PHE:HB2   | 2.16                     | 0.46              |
| 1:A:684:TRP:HZ2  | 1:A:689:CYS:SG    | 2.39                     | 0.46              |
| 1:A:917:LYS:NZ   | 1:A:917:LYS:CB    | 2.78                     | 0.46              |
| 1:A:1007:THR:HB  | 1:A:1152:VAL:HG22 | 1.96                     | 0.46              |
| 1:A:1040:VAL:HA  | 1:A:1098:LEU:HD22 | 1.96                     | 0.46              |
| 1:B:93:MET:O     | 1:B:97:MET:HG3    | 2.16                     | 0.46              |
| 1:B:97:MET:HE1   | 1:B:133:ALA:HB1   | 1.98                     | 0.46              |
| 1:B:1048:GLN:C   | 1:B:1048:GLN:NE2  | 2.73                     | 0.46              |
| 1:B:1200:THR:CG2 | 1:B:1202:MET:H    | 2.28                     | 0.46              |
| 1:A:368:LYS:HZ3  | 1:B:227:GLN:HE22  | 1.62                     | 0.46              |
| 1:A:820:TYR:HD1  | 1:A:1049:PHE:CZ   | 2.34                     | 0.46              |
| 1:B:820:TYR:HD1  | 1:B:1049:PHE:CZ   | 2.34                     | 0.46              |
| 1:A:97:MET:HE1   | 1:A:133:ALA:HB1   | 1.98                     | 0.46              |
| 1:B:184:GLU:CD   | 1:B:256:ARG:HH12  | 2.23                     | 0.46              |
| 1:A:694:GLN:O    | 1:A:698:VAL:HB    | 2.16                     | 0.46              |
| 1:A:1043:GLY:HA2 | 1:A:1084:GLN:NE2  | 2.31                     | 0.46              |
| 1:A:1219:THR:HB  | 1:A:1222:GLN:OE1  | 2.16                     | 0.46              |
| 1:B:152:MET:HE3  | 1:B:303:ARG:HG3   | 1.98                     | 0.45              |
| 1:B:274:VAL:HG23 | 1:B:324:ILE:HD12  | 1.98                     | 0.45              |
| 1:A:280:CYS:HB3  | 1:A:301:LYS:HG2   | 1.99                     | 0.45              |
| 1:A:421:GLN:HA   | 1:A:466:SER:O     | 2.16                     | 0.45              |
| 1:A:644:LYS:N    | 1:A:645:PRO:CD    | 2.79                     | 0.45              |
| 1:A:1010:VAL:O   | 1:B:1188:PHE:HB3  | 2.16                     | 0.45              |
| 1:A:1071:CYS:HA  | 4:A:1235:SF4:S3   | 2.56                     | 0.45              |
| 1:A:1162:GLU:HG3 | 1:B:1171:ILE:HG21 | 1.98                     | 0.45              |
| 1:B:780:TYR:HA   | 1:B:783:ARG:HD2   | 1.99                     | 0.45              |
| 1:B:1074:GLN:O   | 1:B:1133:ARG:HG2  | 2.16                     | 0.45              |
| 1:A:64:GLU:HG3   | 1:A:89:GLY:CA     | 2.45                     | 0.45              |
| 1:A:198:LYS:O    | 1:A:202:GLU:HG3   | 2.17                     | 0.45              |
| 1:A:325:THR:HG23 | 1:A:382:MET:CE    | 2.47                     | 0.45              |
| 1:A:1141:PHE:N   | 1:A:1142:PRO:HD3  | 2.31                     | 0.45              |
| 1:B:87:SER:HA    | 1:B:129:ASP:CB    | 2.46                     | 0.45              |
| 1:B:146:VAL:HG21 | 1:B:179:GLU:O     | 2.16                     | 0.45              |
| 1:B:421:GLN:HA   | 1:B:466:SER:O     | 2.16                     | 0.45              |
| 1:B:1141:PHE:N   | 1:B:1142:PRO:HD3  | 2.31                     | 0.45              |
| 1:A:93:MET:O     | 1:A:97:MET:HG3    | 2.16                     | 0.45              |
| 1:A:208:MET:HE2  | 1:B:833:PHE:HD2   | 1.82                     | 0.45              |
| 1:A:469:ARG:NH2  | 1:A:479:TYR:O     | 2.49                     | 0.45              |
| 1:A:1080:MET:H   | 1:B:1215:ASN:ND2  | 2.14                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1129:MET:HG2 | 1:A:1149:ARG:HE  | 1.80                     | 0.45              |
| 1:B:280:CYS:HB3  | 1:B:301:LYS:HG2  | 1.99                     | 0.45              |
| 1:B:286:VAL:HG12 | 1:B:290:LEU:HD22 | 1.97                     | 0.45              |
| 1:B:390:PHE:CG   | 1:B:403:LEU:HD13 | 2.51                     | 0.45              |
| 1:B:710:LYS:HD2  | 1:B:734:TYR:CE1  | 2.51                     | 0.45              |
| 1:B:755:CYS:HA   | 1:B:756:PRO:HD3  | 1.64                     | 0.45              |
| 1:B:1071:CYS:HA  | 4:B:1242:SF4:S3  | 2.56                     | 0.45              |
| 1:A:617:LYS:HA   | 1:A:617:LYS:HD3  | 1.71                     | 0.45              |
| 1:A:1074:GLN:O   | 1:A:1133:ARG:HG2 | 2.16                     | 0.45              |
| 1:B:198:LYS:O    | 1:B:202:GLU:HG3  | 2.17                     | 0.45              |
| 1:B:469:ARG:NH2  | 1:B:479:TYR:O    | 2.49                     | 0.45              |
| 1:B:1219:THR:HB  | 1:B:1222:GLN:OE1 | 2.16                     | 0.45              |
| 1:A:87:SER:HA    | 1:A:129:ASP:CB   | 2.47                     | 0.45              |
| 1:A:704:ILE:HG12 | 1:A:740:ILE:CD1  | 2.47                     | 0.45              |
| 1:A:790:VAL:HG13 | 1:A:791:LEU:N    | 2.31                     | 0.45              |
| 1:B:684:TRP:HZ2  | 1:B:689:CYS:SG   | 2.39                     | 0.45              |
| 1:B:1059:PHE:HD1 | 1:B:1104:ARG:CD  | 2.30                     | 0.45              |
| 1:A:87:SER:N     | 1:A:129:ASP:OD2  | 2.49                     | 0.45              |
| 1:A:124:PHE:CB   | 1:A:367:SER:HB2  | 2.26                     | 0.45              |
| 1:A:390:PHE:CG   | 1:A:403:LEU:HD13 | 2.51                     | 0.45              |
| 1:A:467:HIS:C    | 1:A:468:LEU:HD23 | 2.42                     | 0.45              |
| 1:A:1198:ASP:OD2 | 1:A:1203:MET:HE3 | 2.17                     | 0.45              |
| 1:B:467:HIS:C    | 1:B:468:LEU:HD23 | 2.42                     | 0.45              |
| 1:B:704:ILE:HG12 | 1:B:740:ILE:CD1  | 2.47                     | 0.45              |
| 1:A:210:PRO:CB   | 1:B:831:ARG:HA   | 2.47                     | 0.45              |
| 1:A:791:LEU:HD23 | 1:A:791:LEU:HA   | 1.84                     | 0.45              |
| 1:B:14:THR:HG21  | 1:B:171:PHE:CE1  | 2.51                     | 0.45              |
| 1:B:173:GLY:O    | 1:B:174:PHE:HB2  | 2.16                     | 0.45              |
| 1:B:512:LEU:HG   | 1:B:514:SER:HB3  | 1.98                     | 0.45              |
| 1:B:790:VAL:HG13 | 1:B:791:LEU:N    | 2.31                     | 0.45              |
| 1:A:780:TYR:HA   | 1:A:783:ARG:HD2  | 1.99                     | 0.45              |
| 1:B:44:ALA:CB    | 1:B:58:ILE:HD11  | 2.47                     | 0.45              |
| 1:B:87:SER:N     | 1:B:129:ASP:OD2  | 2.49                     | 0.45              |
| 1:B:887:ARG:NH2  | 1:B:954:LYS:N    | 2.65                     | 0.45              |
| 1:A:78:GLY:HA2   | 1:A:207:SER:OG   | 2.17                     | 0.45              |
| 1:A:593:LYS:HD3  | 1:A:594:LYS:H    | 1.82                     | 0.45              |
| 1:A:755:CYS:SG   | 1:A:761:ALA:CB   | 3.02                     | 0.45              |
| 1:B:707:VAL:O    | 1:B:736:PHE:HA   | 2.17                     | 0.45              |
| 1:B:1005:THR:HA  | 1:B:1006:PRO:HD3 | 1.71                     | 0.45              |
| 1:A:707:VAL:O    | 1:A:736:PHE:HA   | 2.17                     | 0.44              |
| 1:A:741:ASN:CG   | 1:A:744:ASP:HB2  | 2.42                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:940:GLY:O     | 1:B:941:LEU:C    | 2.60                     | 0.44              |
| 1:B:1043:GLY:HA2  | 1:B:1084:GLN:NE2 | 2.31                     | 0.44              |
| 1:A:596:GLU:O     | 1:A:599:VAL:HB   | 2.18                     | 0.44              |
| 1:A:636:ASN:ND2   | 1:A:672:PHE:CE2  | 2.85                     | 0.44              |
| 1:A:670:SER:HA    | 1:A:673:GLU:OE1  | 2.18                     | 0.44              |
| 1:A:940:GLY:O     | 1:A:941:LEU:C    | 2.60                     | 0.44              |
| 1:A:1108:GLN:H    | 1:A:1108:GLN:HG2 | 1.57                     | 0.44              |
| 1:B:636:ASN:ND2   | 1:B:672:PHE:CE2  | 2.85                     | 0.44              |
| 1:A:1059:PHE:HD1  | 1:A:1104:ARG:CD  | 2.30                     | 0.44              |
| 1:A:44:ALA:CB     | 1:A:58:ILE:HD11  | 2.47                     | 0.44              |
| 1:A:146:VAL:HG21  | 1:A:179:GLU:O    | 2.16                     | 0.44              |
| 1:A:152:MET:HE3   | 1:A:303:ARG:HG3  | 1.98                     | 0.44              |
| 1:A:208:MET:HE1   | 1:B:879:MET:CE   | 2.46                     | 0.44              |
| 1:A:325:THR:HA    | 1:A:359:LEU:O    | 2.18                     | 0.44              |
| 1:B:35:THR:O      | 1:B:36:MET:C     | 2.61                     | 0.44              |
| 1:B:82:THR:HG22   | 1:B:83:THR:N     | 2.26                     | 0.44              |
| 1:B:644:LYS:N     | 1:B:645:PRO:CD   | 2.79                     | 0.44              |
| 1:B:741:ASN:CG    | 1:B:744:ASP:HB2  | 2.42                     | 0.44              |
| 1:A:368:LYS:NZ    | 1:B:227:GLN:NE2  | 2.65                     | 0.44              |
| 1:A:887:ARG:NH2   | 1:A:954:LYS:N    | 2.65                     | 0.44              |
| 1:B:124:PHE:HB3   | 1:B:367:SER:CB   | 2.28                     | 0.44              |
| 1:B:325:THR:HG23  | 1:B:382:MET:CE   | 2.47                     | 0.44              |
| 1:B:35:THR:O      | 1:B:38:GLU:N     | 2.51                     | 0.44              |
| 1:B:64:GLU:OE2    | 5:B:1243:TPP:N1' | 2.51                     | 0.44              |
| 1:A:263:TYR:OH    | 1:A:298:GLY:HA3  | 2.18                     | 0.44              |
| 1:A:331:LYS:HE3   | 1:B:230:GLU:OE2  | 2.17                     | 0.44              |
| 1:A:1219:THR:HG21 | 1:A:1221:GLU:HG2 | 2.00                     | 0.44              |
| 1:B:140:MET:HE3   | 1:B:168:MET:SD   | 2.58                     | 0.44              |
| 1:B:523:ASP:HA    | 1:B:531:LYS:HZ1  | 1.78                     | 0.44              |
| 1:B:593:LYS:HD3   | 1:B:594:LYS:H    | 1.82                     | 0.44              |
| 1:B:746:MET:HB3   | 1:B:813:SER:OG   | 2.18                     | 0.44              |
| 1:B:1082:LYS:HD3  | 1:B:1082:LYS:HA  | 1.84                     | 0.44              |
| 1:B:1219:THR:HG21 | 1:B:1221:GLU:HG2 | 2.00                     | 0.44              |
| 1:A:512:LEU:HG    | 1:A:514:SER:HB3  | 1.98                     | 0.44              |
| 1:A:890:LEU:CD1   | 1:A:945:ILE:HG23 | 2.45                     | 0.44              |
| 1:B:263:TYR:OH    | 1:B:298:GLY:HA3  | 2.18                     | 0.44              |
| 1:B:698:VAL:HG22  | 1:B:1084:GLN:CD  | 2.43                     | 0.44              |
| 1:A:805:LEU:HD22  | 1:A:829:GLY:HA3  | 2.00                     | 0.44              |
| 1:A:843:ILE:HG13  | 1:A:996:ASN:OD1  | 2.18                     | 0.44              |
| 1:A:1005:THR:HA   | 1:A:1006:PRO:HD3 | 1.71                     | 0.44              |
| 1:B:596:GLU:O     | 1:B:599:VAL:HB   | 2.18                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:805:LEU:HD22  | 1:B:829:GLY:HA3  | 2.00                     | 0.44              |
| 1:A:140:MET:HE3   | 1:A:168:MET:SD   | 2.58                     | 0.43              |
| 1:B:803:GLU:O     | 1:B:805:LEU:HD13 | 2.18                     | 0.43              |
| 1:B:867:SER:HB2   | 1:B:875:TYR:CD2  | 2.53                     | 0.43              |
| 1:B:843:ILE:HG13  | 1:B:996:ASN:OD1  | 2.18                     | 0.43              |
| 1:B:1000:GLN:HE21 | 1:B:1000:GLN:HB2 | 1.67                     | 0.43              |
| 1:B:1198:ASP:OD2  | 1:B:1203:MET:HE3 | 2.17                     | 0.43              |
| 1:A:746:MET:HB3   | 1:A:813:SER:OG   | 2.18                     | 0.43              |
| 1:A:754:ILE:O     | 1:A:755:CYS:C    | 2.61                     | 0.43              |
| 1:B:325:THR:HA    | 1:B:359:LEU:O    | 2.18                     | 0.43              |
| 1:B:679:ILE:HD13  | 1:B:679:ILE:HA   | 1.90                     | 0.43              |
| 1:A:64:GLU:OE2    | 5:A:1236:TPP:N1' | 2.51                     | 0.43              |
| 1:A:650:GLN:NE2   | 1:A:653:LYS:NZ   | 2.66                     | 0.43              |
| 1:A:821:VAL:O     | 1:A:825:THR:HG23 | 2.18                     | 0.43              |
| 1:B:78:GLY:HA2    | 1:B:207:SER:OG   | 2.17                     | 0.43              |
| 1:B:490:HIS:CD2   | 1:B:490:HIS:N    | 2.86                     | 0.43              |
| 1:B:650:GLN:NE2   | 1:B:653:LYS:NZ   | 2.66                     | 0.43              |
| 1:B:670:SER:HA    | 1:B:673:GLU:OE1  | 2.18                     | 0.43              |
| 1:B:1180:GLY:O    | 1:B:1181:LYS:HD2 | 2.19                     | 0.43              |
| 1:A:35:THR:O      | 1:A:38:GLU:N     | 2.51                     | 0.43              |
| 1:A:290:LEU:O     | 1:A:293:LYS:HB2  | 2.19                     | 0.43              |
| 1:A:593:LYS:CG    | 1:A:594:LYS:H    | 2.31                     | 0.43              |
| 1:B:290:LEU:O     | 1:B:293:LYS:HB2  | 2.19                     | 0.43              |
| 1:A:1104:ARG:O    | 1:A:1107:ALA:HB3 | 2.18                     | 0.43              |
| 1:A:1180:GLY:O    | 1:A:1181:LYS:HD2 | 2.19                     | 0.43              |
| 1:A:317:LEU:HD21  | 1:A:321:ALA:CB   | 2.49                     | 0.43              |
| 1:B:591:TYR:HA    | 1:B:593:LYS:HG2  | 2.00                     | 0.43              |
| 1:B:1104:ARG:O    | 1:B:1107:ALA:HB3 | 2.18                     | 0.43              |
| 1:A:11:ASN:HD21   | 1:A:112:THR:HG21 | 1.84                     | 0.43              |
| 1:A:521:ASP:O     | 1:A:522:MET:C    | 2.62                     | 0.43              |
| 1:A:552:ASP:C     | 1:A:554:GLY:H    | 2.27                     | 0.43              |
| 1:A:687:GLU:H     | 1:A:687:GLU:HG3  | 1.65                     | 0.43              |
| 1:A:831:ARG:HA    | 1:B:210:PRO:HB2  | 2.01                     | 0.43              |
| 1:A:1217:ALA:HB2  | 1:B:679:ILE:HB   | 2.01                     | 0.43              |
| 1:B:1227:SER:C    | 1:B:1229:ARG:H   | 2.27                     | 0.43              |
| 1:A:693:ASN:HD21  | 1:A:736:PHE:HZ   | 1.63                     | 0.43              |
| 1:A:698:VAL:HG22  | 1:A:1084:GLN:CD  | 2.43                     | 0.43              |
| 1:A:698:VAL:O     | 1:A:700:PRO:HD3  | 2.19                     | 0.43              |
| 1:A:867:SER:HB2   | 1:A:875:TYR:CD2  | 2.53                     | 0.43              |
| 1:B:226:PHE:O     | 1:B:226:PHE:CD1  | 2.72                     | 0.43              |
| 1:B:509:THR:HA    | 1:B:540:LYS:HB2  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:593:LYS:HD2  | 1:B:598:ILE:HG13 | 2.01                     | 0.43              |
| 1:B:317:LEU:HD21 | 1:B:321:ALA:CB   | 2.49                     | 0.43              |
| 1:B:374:MET:O    | 1:B:377:SER:HB3  | 2.18                     | 0.43              |
| 1:B:698:VAL:O    | 1:B:700:PRO:HD3  | 2.19                     | 0.43              |
| 1:A:370:PHE:CZ   | 1:A:375:VAL:HG22 | 2.54                     | 0.42              |
| 1:A:422:PHE:CE1  | 1:A:468:LEU:HG   | 2.54                     | 0.42              |
| 1:B:212:HIS:O    | 1:B:212:HIS:CG   | 2.72                     | 0.42              |
| 1:B:346:SER:O    | 1:B:350:GLU:HB3  | 2.19                     | 0.42              |
| 1:B:370:PHE:CZ   | 1:B:375:VAL:HG22 | 2.54                     | 0.42              |
| 1:A:19:TYR:CD1   | 1:A:19:TYR:C     | 2.97                     | 0.42              |
| 1:A:208:MET:HE2  | 1:B:833:PHE:CD2  | 2.54                     | 0.42              |
| 1:A:630:LYS:H    | 1:A:630:LYS:HG3  | 1.57                     | 0.42              |
| 1:A:1094:GLY:HA3 | 1:A:1120:PRO:HG3 | 2.00                     | 0.42              |
| 1:A:1227:SER:C   | 1:A:1229:ARG:H   | 2.27                     | 0.42              |
| 1:B:19:TYR:CD1   | 1:B:19:TYR:C     | 2.97                     | 0.42              |
| 1:B:154:LEU:HD13 | 1:B:250:VAL:CG2  | 2.49                     | 0.42              |
| 1:B:266:ALA:HA   | 1:B:267:PRO:HD3  | 1.91                     | 0.42              |
| 1:B:455:TYR:HB3  | 1:B:456:ASP:H    | 1.64                     | 0.42              |
| 1:B:511:VAL:CG2  | 1:B:563:MET:HE1  | 2.50                     | 0.42              |
| 1:B:821:VAL:O    | 1:B:825:THR:HG23 | 2.18                     | 0.42              |
| 1:A:154:LEU:HD13 | 1:A:250:VAL:CG2  | 2.49                     | 0.42              |
| 1:A:509:THR:HA   | 1:A:540:LYS:HB2  | 2.01                     | 0.42              |
| 1:A:511:VAL:HA   | 1:A:542:TYR:O    | 2.19                     | 0.42              |
| 1:A:792:PRO:O    | 1:A:793:ARG:C    | 2.63                     | 0.42              |
| 1:A:1205:ARG:HA  | 1:A:1205:ARG:HD3 | 1.82                     | 0.42              |
| 1:B:390:PHE:HA   | 1:B:401:THR:O    | 2.19                     | 0.42              |
| 1:B:554:GLY:CA   | 1:B:601:MET:HE2  | 2.40                     | 0.42              |
| 1:B:593:LYS:CG   | 1:B:594:LYS:H    | 2.31                     | 0.42              |
| 1:B:897:ALA:HB3  | 1:B:910:LEU:HD21 | 2.01                     | 0.42              |
| 1:A:266:ALA:HA   | 1:A:267:PRO:HD3  | 1.91                     | 0.42              |
| 1:A:346:SER:O    | 1:A:350:GLU:HB3  | 2.19                     | 0.42              |
| 1:A:490:HIS:N    | 1:A:490:HIS:CD2  | 2.86                     | 0.42              |
| 1:B:64:GLU:CG    | 1:B:89:GLY:HA2   | 2.48                     | 0.42              |
| 1:B:154:LEU:CD2  | 1:B:158:LEU:HD11 | 2.49                     | 0.42              |
| 1:B:342:LEU:HD12 | 1:B:342:LEU:HA   | 1.82                     | 0.42              |
| 1:B:472:GLU:H    | 1:B:472:GLU:HG2  | 1.55                     | 0.42              |
| 1:B:754:ILE:O    | 1:B:755:CYS:C    | 2.61                     | 0.42              |
| 1:A:307:PRO:HA   | 1:B:334:GLY:O    | 2.19                     | 0.42              |
| 1:A:591:TYR:HA   | 1:A:593:LYS:HG2  | 2.00                     | 0.42              |
| 1:A:897:ALA:HB3  | 1:A:910:LEU:HD21 | 2.01                     | 0.42              |
| 1:B:536:ASN:ND2  | 1:B:623:LYS:HG2  | 2.34                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:599:VAL:O    | 1:B:602:ASN:HB2   | 2.20                     | 0.42              |
| 1:A:35:THR:O     | 1:A:36:MET:C      | 2.61                     | 0.42              |
| 1:A:390:PHE:HA   | 1:A:401:THR:O     | 2.19                     | 0.42              |
| 1:A:803:GLU:O    | 1:A:805:LEU:HD13  | 2.18                     | 0.42              |
| 1:B:5:MET:HE1    | 1:B:184:GLU:HB2   | 2.02                     | 0.42              |
| 1:B:736:PHE:CD2  | 1:B:801:PHE:HZ    | 2.37                     | 0.42              |
| 1:B:792:PRO:O    | 1:B:793:ARG:C     | 2.63                     | 0.42              |
| 1:B:1094:GLY:HA3 | 1:B:1120:PRO:HG3  | 2.00                     | 0.42              |
| 1:B:1123:SER:O   | 1:B:1124:VAL:C    | 2.63                     | 0.42              |
| 1:A:5:MET:HE1    | 1:A:184:GLU:HB2   | 2.02                     | 0.42              |
| 1:A:374:MET:O    | 1:A:377:SER:HB3   | 2.18                     | 0.42              |
| 1:A:390:PHE:CD2  | 1:A:403:LEU:HD22  | 2.54                     | 0.42              |
| 1:A:467:HIS:CE1  | 1:A:480:LEU:HD22  | 2.55                     | 0.42              |
| 1:A:1082:LYS:HD3 | 1:A:1082:LYS:HA   | 1.84                     | 0.42              |
| 1:B:11:ASN:HD21  | 1:B:112:THR:HG21  | 1.84                     | 0.42              |
| 1:B:325:THR:HG22 | 1:B:382:MET:SD    | 2.60                     | 0.42              |
| 1:B:390:PHE:CD2  | 1:B:403:LEU:HD22  | 2.54                     | 0.42              |
| 1:B:596:GLU:O    | 1:B:597:LYS:C     | 2.62                     | 0.42              |
| 1:B:840:CYS:O    | 1:B:844:TRP:CD1   | 2.72                     | 0.42              |
| 1:B:1108:GLN:H   | 1:B:1108:GLN:HG2  | 1.57                     | 0.42              |
| 1:A:226:PHE:O    | 1:A:226:PHE:CD1   | 2.72                     | 0.42              |
| 1:A:511:VAL:CG2  | 1:A:563:MET:HE1   | 2.50                     | 0.42              |
| 1:A:513:ASN:HA   | 1:A:544:ILE:O     | 2.20                     | 0.42              |
| 1:A:736:PHE:CD2  | 1:A:801:PHE:HZ    | 2.37                     | 0.42              |
| 1:A:941:LEU:HA   | 1:A:941:LEU:HD23  | 1.86                     | 0.42              |
| 1:A:976:HIS:HE1  | 1:B:60:GLU:O      | 2.03                     | 0.42              |
| 1:B:338:ASP:HB3  | 1:B:339:PRO:CD    | 2.50                     | 0.42              |
| 1:B:465:ILE:HG13 | 1:B:467:HIS:HE1   | 1.84                     | 0.42              |
| 1:B:552:ASP:C    | 1:B:554:GLY:H     | 2.27                     | 0.42              |
| 1:B:687:GLU:H    | 1:B:687:GLU:HG3   | 1.65                     | 0.42              |
| 1:B:1149:ARG:HG3 | 1:B:1149:ARG:NH1  | 2.15                     | 0.42              |
| 1:A:64:GLU:CG    | 1:A:89:GLY:HA2    | 2.48                     | 0.42              |
| 1:A:154:LEU:CD2  | 1:A:158:LEU:HD11  | 2.49                     | 0.42              |
| 1:A:212:HIS:O    | 1:A:212:HIS:CG    | 2.72                     | 0.42              |
| 1:A:696:ALA:O    | 1:A:822:ARG:NH2   | 2.53                     | 0.42              |
| 1:A:840:CYS:O    | 1:A:844:TRP:CD1   | 2.72                     | 0.42              |
| 1:B:317:LEU:HD21 | 1:B:321:ALA:HB3   | 2.02                     | 0.42              |
| 1:B:536:ASN:HD22 | 1:B:623:LYS:HZ3   | 1.66                     | 0.42              |
| 1:B:780:TYR:CE2  | 1:B:784:ILE:HD11  | 2.55                     | 0.42              |
| 1:B:1132:ASN:ND2 | 1:B:1139:ARG:HH12 | 2.11                     | 0.42              |
| 1:A:465:ILE:HG13 | 1:A:467:HIS:HE1   | 1.84                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1082:LYS:NZ  | 1:B:1219:THR:HG21 | 2.34                     | 0.42              |
| 1:B:32:PRO:HB3   | 1:B:174:PHE:CE2   | 2.55                     | 0.42              |
| 1:B:513:ASN:HA   | 1:B:544:ILE:O     | 2.20                     | 0.42              |
| 1:B:715:VAL:C    | 1:B:717:ALA:N     | 2.77                     | 0.42              |
| 1:A:32:PRO:HB3   | 1:A:174:PHE:CE2   | 2.55                     | 0.41              |
| 1:A:227:GLN:HE22 | 1:B:368:LYS:HZ3   | 1.68                     | 0.41              |
| 1:A:780:TYR:CE2  | 1:A:784:ILE:HD11  | 2.55                     | 0.41              |
| 1:A:965:TRP:CZ3  | 1:A:966:ALA:HB2   | 2.55                     | 0.41              |
| 1:B:197:GLN:H    | 1:B:197:GLN:HG2   | 1.64                     | 0.41              |
| 1:B:467:HIS:CE1  | 1:B:480:LEU:HD22  | 2.55                     | 0.41              |
| 1:B:630:LYS:H    | 1:B:630:LYS:HG3   | 1.57                     | 0.41              |
| 1:B:748:CYS:SG   | 1:B:750:ASN:HB2   | 2.60                     | 0.41              |
| 1:B:837:ALA:HB2  | 1:B:872:ALA:CB    | 2.50                     | 0.41              |
| 1:A:317:LEU:HD21 | 1:A:321:ALA:HB3   | 2.02                     | 0.41              |
| 1:A:660:GLU:O    | 1:A:661:ALA:C     | 2.63                     | 0.41              |
| 1:A:837:ALA:HB2  | 1:A:872:ALA:CB    | 2.50                     | 0.41              |
| 1:A:1209:GLY:O   | 1:B:429:GLY:HA2   | 2.19                     | 0.41              |
| 1:B:227:GLN:NE2  | 1:B:227:GLN:H     | 2.18                     | 0.41              |
| 1:B:1059:PHE:CD1 | 1:B:1104:ARG:HD3  | 2.55                     | 0.41              |
| 1:A:208:MET:HE1  | 1:B:879:MET:HE1   | 2.01                     | 0.41              |
| 1:A:748:CYS:SG   | 1:A:750:ASN:HB2   | 2.60                     | 0.41              |
| 1:A:1132:ASN:ND2 | 1:A:1139:ARG:HH12 | 2.11                     | 0.41              |
| 1:B:23:GLU:CD    | 1:B:204:ARG:HH22  | 2.28                     | 0.41              |
| 1:B:371:SER:HB2  | 1:B:372:PRO:CD    | 2.51                     | 0.41              |
| 1:B:897:ALA:HA   | 1:B:941:LEU:HD13  | 2.03                     | 0.41              |
| 1:B:965:TRP:CZ3  | 1:B:966:ALA:HB2   | 2.55                     | 0.41              |
| 1:B:1149:ARG:CG  | 1:B:1149:ARG:NH1  | 2.80                     | 0.41              |
| 1:A:23:GLU:CD    | 1:A:204:ARG:HH22  | 2.28                     | 0.41              |
| 1:A:238:LYS:O    | 1:A:242:ILE:HG13  | 2.20                     | 0.41              |
| 1:A:536:ASN:HA   | 1:A:623:LYS:HZ3   | 1.85                     | 0.41              |
| 1:A:596:GLU:O    | 1:A:597:LYS:C     | 2.62                     | 0.41              |
| 1:A:700:PRO:HB3  | 1:A:819:PRO:HD3   | 2.02                     | 0.41              |
| 1:A:743:LEU:HD23 | 1:A:743:LEU:HA    | 1.73                     | 0.41              |
| 1:A:1123:SER:O   | 1:A:1124:VAL:C    | 2.63                     | 0.41              |
| 1:A:1149:ARG:HG3 | 1:A:1149:ARG:NH1  | 2.15                     | 0.41              |
| 1:B:314:PHE:C    | 1:B:316:ALA:H     | 2.27                     | 0.41              |
| 1:B:491:ASN:HA   | 1:B:492:PRO:HD2   | 1.84                     | 0.41              |
| 1:B:644:LYS:HB3  | 1:B:645:PRO:HD3   | 2.02                     | 0.41              |
| 1:B:1001:SER:HB2 | 1:B:1011:ALA:HB3  | 2.01                     | 0.41              |
| 1:A:536:ASN:ND2  | 1:A:623:LYS:HG2   | 2.34                     | 0.41              |
| 1:A:593:LYS:HD2  | 1:A:598:ILE:HG13  | 2.01                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1200:THR:HA   | 1:A:1201:PRO:HD3 | 1.83                     | 0.41              |
| 1:A:371:SER:HB2   | 1:A:372:PRO:CD   | 2.50                     | 0.41              |
| 1:A:599:VAL:O     | 1:A:602:ASN:HB2  | 2.20                     | 0.41              |
| 1:A:1215:ASN:HD21 | 1:B:1080:MET:H   | 1.68                     | 0.41              |
| 1:B:696:ALA:O     | 1:B:822:ARG:NH2  | 2.53                     | 0.41              |
| 1:B:721:PHE:HD1   | 1:B:777:ASN:ND2  | 2.18                     | 0.41              |
| 1:A:86:ALA:O      | 1:A:87:SER:C     | 2.64                     | 0.41              |
| 1:A:210:PRO:O     | 1:B:860:GLN:HB2  | 2.19                     | 0.41              |
| 1:A:338:ASP:HB3   | 1:A:339:PRO:CD   | 2.50                     | 0.41              |
| 1:A:349:VAL:HG12  | 1:B:349:VAL:HG12 | 2.03                     | 0.41              |
| 1:A:715:VAL:C     | 1:A:717:ALA:N    | 2.77                     | 0.41              |
| 1:A:1001:SER:HB2  | 1:A:1011:ALA:HB3 | 2.01                     | 0.41              |
| 1:B:700:PRO:HB3   | 1:B:819:PRO:HD3  | 2.02                     | 0.41              |
| 1:A:477:SER:HB3   | 1:A:479:TYR:CE1  | 2.55                     | 0.41              |
| 1:A:593:LYS:CD    | 1:A:594:LYS:H    | 2.34                     | 0.41              |
| 1:A:897:ALA:HA    | 1:A:941:LEU:HD13 | 2.03                     | 0.41              |
| 1:A:1137:LEU:HD23 | 1:A:1137:LEU:HA  | 1.90                     | 0.41              |
| 1:B:86:ALA:O      | 1:B:87:SER:C     | 2.64                     | 0.41              |
| 1:B:477:SER:HB3   | 1:B:479:TYR:CE1  | 2.55                     | 0.41              |
| 1:B:511:VAL:HA    | 1:B:542:TYR:O    | 2.19                     | 0.41              |
| 1:B:617:LYS:HA    | 1:B:617:LYS:HD3  | 1.71                     | 0.41              |
| 1:B:718:PRO:HB2   | 1:B:777:ASN:HD21 | 1.86                     | 0.41              |
| 5:B:1243:TPP:HN42 | 5:B:1243:TPP:C2  | 2.33                     | 0.41              |
| 1:A:234:PRO:CA    | 1:A:237:LEU:HD12 | 2.44                     | 0.41              |
| 1:A:314:PHE:C     | 1:A:316:ALA:H    | 2.27                     | 0.41              |
| 1:A:325:THR:HG23  | 1:A:382:MET:HE2  | 2.03                     | 0.41              |
| 1:A:368:LYS:NZ    | 1:B:223:ASP:O    | 2.54                     | 0.41              |
| 1:A:461:GLY:H     | 1:B:1214:GLN:CD  | 2.29                     | 0.41              |
| 1:A:644:LYS:HB3   | 1:A:645:PRO:HD3  | 2.02                     | 0.41              |
| 1:A:804:PRO:HG3   | 1:A:826:GLN:HE21 | 1.86                     | 0.41              |
| 1:A:879:MET:CE    | 1:B:208:MET:HE1  | 2.51                     | 0.41              |
| 1:B:226:PHE:CD1   | 1:B:226:PHE:C    | 2.99                     | 0.41              |
| 1:B:325:THR:HG23  | 1:B:382:MET:HE2  | 2.03                     | 0.41              |
| 1:B:593:LYS:CD    | 1:B:594:LYS:H    | 2.34                     | 0.41              |
| 1:B:660:GLU:O     | 1:B:661:ALA:C    | 2.63                     | 0.41              |
| 5:B:1243:TPP:H2   | 5:B:1243:TPP:N4' | 2.36                     | 0.41              |
| 1:A:605:ALA:O     | 1:A:609:ALA:HB2  | 2.21                     | 0.41              |
| 1:A:821:VAL:HG21  | 1:A:844:TRP:HH2  | 1.86                     | 0.41              |
| 1:A:875:TYR:CE1   | 1:B:73:GLY:HA2   | 2.56                     | 0.41              |
| 1:A:1177:PRO:O    | 1:A:1178:ALA:HB2 | 2.21                     | 0.41              |
| 1:B:346:SER:O     | 1:B:350:GLU:CB   | 2.69                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:605:ALA:O     | 1:B:609:ALA:HB2  | 2.21                     | 0.41              |
| 1:B:619:PRO:HB2   | 1:B:621:SER:HB3  | 2.03                     | 0.41              |
| 1:B:1177:PRO:O    | 1:B:1178:ALA:HB2 | 2.21                     | 0.41              |
| 1:A:697:PHE:HD2   | 1:A:800:GLN:HE21 | 1.67                     | 0.40              |
| 5:A:1236:TPP:H2   | 5:A:1236:TPP:N4' | 2.36                     | 0.40              |
| 1:B:853:TYR:CE2   | 1:B:864:TRP:NE1  | 2.89                     | 0.40              |
| 1:A:24:VAL:CG1    | 1:B:881:MET:HE2  | 2.46                     | 0.40              |
| 1:A:96:ASN:O      | 1:A:99:LYS:N     | 2.55                     | 0.40              |
| 1:A:226:PHE:CD1   | 1:A:226:PHE:C    | 2.99                     | 0.40              |
| 5:A:1236:TPP:HN42 | 5:A:1236:TPP:C2  | 2.33                     | 0.40              |
| 1:B:96:ASN:O      | 1:B:99:LYS:N     | 2.55                     | 0.40              |
| 1:B:238:LYS:O     | 1:B:242:ILE:HG13 | 2.20                     | 0.40              |
| 1:B:273:ILE:HD13  | 1:B:273:ILE:HG21 | 1.63                     | 0.40              |
| 1:B:755:CYS:HA    | 4:B:1240:SF4:S1  | 2.61                     | 0.40              |
| 1:B:893:LEU:HD12  | 1:B:893:LEU:HA   | 1.88                     | 0.40              |
| 1:A:342:LEU:HD12  | 1:A:342:LEU:HA   | 1.82                     | 0.40              |
| 1:A:619:PRO:HB2   | 1:A:621:SER:HB3  | 2.03                     | 0.40              |
| 1:A:721:PHE:HD1   | 1:A:777:ASN:ND2  | 2.18                     | 0.40              |
| 1:A:853:TYR:CE2   | 1:A:864:TRP:NE1  | 2.89                     | 0.40              |
| 1:A:1146:LYS:HA   | 1:A:1149:ARG:NH1 | 2.37                     | 0.40              |
| 1:B:755:CYS:SG    | 1:B:761:ALA:CB   | 3.02                     | 0.40              |
| 1:A:5:MET:CE      | 1:A:184:GLU:HB2  | 2.52                     | 0.40              |
| 1:A:693:ASN:O     | 1:A:697:PHE:HB2  | 2.22                     | 0.40              |
| 1:A:755:CYS:HA    | 4:A:1233:SF4:S1  | 2.61                     | 0.40              |
| 1:B:388:ASN:OD1   | 1:B:389:HIS:N    | 2.54                     | 0.40              |
| 1:A:718:PRO:HB2   | 1:A:777:ASN:HD21 | 1.86                     | 0.40              |
| 1:A:856:ASN:HD21  | 1:A:860:GLN:HG3  | 1.87                     | 0.40              |
| 1:A:1118:LYS:HE3  | 1:A:1118:LYS:HB2 | 1.94                     | 0.40              |
| 1:B:811:ALA:HB2   | 1:B:844:TRP:CB   | 2.52                     | 0.40              |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 1:A:292:ALA:N  | 1:B:634:MET:CE[3_445] | 2.01                     | 0.19              |
| 1:A:292:ALA:CA | 1:B:634:MET:CE[3_445] | 2.05                     | 0.15              |
| 1:A:291:ALA:C  | 1:B:634:MET:CE[3_445] | 2.12                     | 0.08              |
| 1:A:291:ALA:O  | 1:B:634:MET:CE[3_445] | 2.18                     | 0.02              |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|----------|-------------|----|
| 1   | A     | 1229/1231 (100%) | 1101 (90%) | 103 (8%) | 25 (2%)  | 6           | 28 |
| 1   | B     | 1229/1231 (100%) | 1102 (90%) | 102 (8%) | 25 (2%)  | 6           | 28 |
| All | All   | 2458/2462 (100%) | 2203 (90%) | 205 (8%) | 50 (2%)  | 6           | 28 |

All (50) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 87   | SER  |
| 1   | A     | 218  | THR  |
| 1   | A     | 595  | GLY  |
| 1   | A     | 626  | PRO  |
| 1   | A     | 627  | ALA  |
| 1   | A     | 1124 | VAL  |
| 1   | A     | 1178 | ALA  |
| 1   | A     | 1231 | LYS  |
| 1   | B     | 87   | SER  |
| 1   | B     | 218  | THR  |
| 1   | B     | 595  | GLY  |
| 1   | B     | 626  | PRO  |
| 1   | B     | 627  | ALA  |
| 1   | B     | 1124 | VAL  |
| 1   | B     | 1178 | ALA  |
| 1   | B     | 1231 | LYS  |
| 1   | A     | 711  | GLU  |
| 1   | A     | 940  | GLY  |
| 1   | A     | 941  | LEU  |
| 1   | A     | 993  | VAL  |
| 1   | A     | 996  | ASN  |
| 1   | A     | 1181 | LYS  |
| 1   | B     | 711  | GLU  |
| 1   | B     | 940  | GLY  |
| 1   | B     | 941  | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 993  | VAL  |
| 1   | B     | 996  | ASN  |
| 1   | B     | 1181 | LYS  |
| 1   | A     | 356  | PRO  |
| 1   | A     | 903  | SER  |
| 1   | A     | 1174 | SER  |
| 1   | B     | 356  | PRO  |
| 1   | B     | 903  | SER  |
| 1   | B     | 1174 | SER  |
| 1   | A     | 221  | ASN  |
| 1   | A     | 353  | GLU  |
| 1   | A     | 364  | GLY  |
| 1   | A     | 691  | GLN  |
| 1   | A     | 1182 | ALA  |
| 1   | B     | 221  | ASN  |
| 1   | B     | 353  | GLU  |
| 1   | B     | 364  | GLY  |
| 1   | B     | 691  | GLN  |
| 1   | B     | 1182 | ALA  |
| 1   | A     | 576  | PHE  |
| 1   | A     | 599  | VAL  |
| 1   | B     | 576  | PHE  |
| 1   | B     | 599  | VAL  |
| 1   | A     | 1179 | GLY  |
| 1   | B     | 1179 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed         | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|------------------|------------|-----------|-------------|----|
| 1   | A     | 978/978 (100%)   | 818 (84%)  | 160 (16%) | 2           | 12 |
| 1   | B     | 978/978 (100%)   | 818 (84%)  | 160 (16%) | 2           | 12 |
| All | All   | 1956/1956 (100%) | 1636 (84%) | 320 (16%) | 2           | 12 |

All (320) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | THR  |
| 1   | A     | 11  | ASN  |
| 1   | A     | 12  | THR  |
| 1   | A     | 14  | THR  |
| 1   | A     | 27  | ILE  |
| 1   | A     | 58  | ILE  |
| 1   | A     | 64  | GLU  |
| 1   | A     | 82  | THR  |
| 1   | A     | 95  | PRO  |
| 1   | A     | 111 | VAL  |
| 1   | A     | 121 | LEU  |
| 1   | A     | 134 | ARG  |
| 1   | A     | 141 | LEU  |
| 1   | A     | 152 | MET  |
| 1   | A     | 154 | LEU  |
| 1   | A     | 175 | ARG  |
| 1   | A     | 180 | ILE  |
| 1   | A     | 184 | GLU  |
| 1   | A     | 194 | LEU  |
| 1   | A     | 198 | LYS  |
| 1   | A     | 204 | ARG  |
| 1   | A     | 206 | LYS  |
| 1   | A     | 211 | GLU  |
| 1   | A     | 213 | PRO  |
| 1   | A     | 215 | VAL  |
| 1   | A     | 218 | THR  |
| 1   | A     | 227 | GLN  |
| 1   | A     | 248 | GLN  |
| 1   | A     | 257 | SER  |
| 1   | A     | 260 | LEU  |
| 1   | A     | 273 | ILE  |
| 1   | A     | 279 | SER  |
| 1   | A     | 287 | ILE  |
| 1   | A     | 290 | LEU  |
| 1   | A     | 302 | VAL  |
| 1   | A     | 303 | ARG  |
| 1   | A     | 317 | LEU  |
| 1   | A     | 324 | ILE  |
| 1   | A     | 325 | THR  |
| 1   | A     | 328 | ASP  |
| 1   | A     | 331 | LYS  |
| 1   | A     | 342 | LEU  |
| 1   | A     | 349 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 351 | ARG  |
| 1   | A     | 357 | LYS  |
| 1   | A     | 359 | LEU  |
| 1   | A     | 365 | LEU  |
| 1   | A     | 367 | SER  |
| 1   | A     | 392 | VAL  |
| 1   | A     | 398 | VAL  |
| 1   | A     | 399 | THR  |
| 1   | A     | 403 | LEU  |
| 1   | A     | 415 | LYS  |
| 1   | A     | 439 | LYS  |
| 1   | A     | 454 | SER  |
| 1   | A     | 460 | SER  |
| 1   | A     | 463 | ILE  |
| 1   | A     | 465 | ILE  |
| 1   | A     | 468 | LEU  |
| 1   | A     | 472 | GLU  |
| 1   | A     | 482 | ASN  |
| 1   | A     | 501 | LEU  |
| 1   | A     | 509 | THR  |
| 1   | A     | 511 | VAL  |
| 1   | A     | 512 | LEU  |
| 1   | A     | 514 | SER  |
| 1   | A     | 517 | SER  |
| 1   | A     | 532 | ARG  |
| 1   | A     | 538 | LYS  |
| 1   | A     | 570 | LEU  |
| 1   | A     | 582 | LEU  |
| 1   | A     | 583 | LEU  |
| 1   | A     | 593 | LYS  |
| 1   | A     | 613 | LEU  |
| 1   | A     | 617 | LYS  |
| 1   | A     | 621 | SER  |
| 1   | A     | 628 | GLU  |
| 1   | A     | 629 | THR  |
| 1   | A     | 630 | LYS  |
| 1   | A     | 635 | THR  |
| 1   | A     | 637 | GLU  |
| 1   | A     | 643 | VAL  |
| 1   | A     | 654 | LEU  |
| 1   | A     | 656 | VAL  |
| 1   | A     | 673 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 677 | VAL  |
| 1   | A     | 681 | VAL  |
| 1   | A     | 683 | GLN  |
| 1   | A     | 687 | GLU  |
| 1   | A     | 698 | VAL  |
| 1   | A     | 702 | SER  |
| 1   | A     | 710 | LYS  |
| 1   | A     | 714 | LEU  |
| 1   | A     | 715 | VAL  |
| 1   | A     | 718 | PRO  |
| 1   | A     | 720 | ASN  |
| 1   | A     | 725 | GLU  |
| 1   | A     | 730 | GLU  |
| 1   | A     | 737 | ARG  |
| 1   | A     | 741 | ASN  |
| 1   | A     | 771 | ARG  |
| 1   | A     | 778 | LEU  |
| 1   | A     | 783 | ARG  |
| 1   | A     | 800 | GLN  |
| 1   | A     | 808 | PHE  |
| 1   | A     | 821 | VAL  |
| 1   | A     | 823 | VAL  |
| 1   | A     | 851 | MET  |
| 1   | A     | 854 | LYS  |
| 1   | A     | 857 | ARG  |
| 1   | A     | 858 | LEU  |
| 1   | A     | 874 | GLU  |
| 1   | A     | 883 | MET  |
| 1   | A     | 887 | ARG  |
| 1   | A     | 910 | LEU  |
| 1   | A     | 914 | LEU  |
| 1   | A     | 917 | LYS  |
| 1   | A     | 921 | ILE  |
| 1   | A     | 930 | LEU  |
| 1   | A     | 941 | LEU  |
| 1   | A     | 942 | LEU  |
| 1   | A     | 949 | SER  |
| 1   | A     | 953 | THR  |
| 1   | A     | 954 | LYS  |
| 1   | A     | 955 | LYS  |
| 1   | A     | 986 | VAL  |
| 1   | A     | 997 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1001 | SER  |
| 1   | A     | 1002 | SER  |
| 1   | A     | 1029 | VAL  |
| 1   | A     | 1048 | GLN  |
| 1   | A     | 1064 | LEU  |
| 1   | A     | 1074 | GLN  |
| 1   | A     | 1104 | ARG  |
| 1   | A     | 1105 | LEU  |
| 1   | A     | 1108 | GLN  |
| 1   | A     | 1110 | LYS  |
| 1   | A     | 1118 | LYS  |
| 1   | A     | 1124 | VAL  |
| 1   | A     | 1126 | GLU  |
| 1   | A     | 1136 | VAL  |
| 1   | A     | 1137 | LEU  |
| 1   | A     | 1146 | LYS  |
| 1   | A     | 1149 | ARG  |
| 1   | A     | 1166 | MET  |
| 1   | A     | 1170 | ASN  |
| 1   | A     | 1171 | ILE  |
| 1   | A     | 1173 | GLU  |
| 1   | A     | 1181 | LYS  |
| 1   | A     | 1185 | SER  |
| 1   | A     | 1186 | VAL  |
| 1   | A     | 1196 | THR  |
| 1   | A     | 1197 | ARG  |
| 1   | A     | 1199 | ASP  |
| 1   | A     | 1200 | THR  |
| 1   | A     | 1205 | ARG  |
| 1   | A     | 1219 | THR  |
| 1   | A     | 1223 | GLN  |
| 1   | A     | 1225 | ASP  |
| 1   | A     | 1232 | LYS  |
| 1   | B     | 7    | THR  |
| 1   | B     | 11   | ASN  |
| 1   | B     | 12   | THR  |
| 1   | B     | 14   | THR  |
| 1   | B     | 27   | ILE  |
| 1   | B     | 58   | ILE  |
| 1   | B     | 64   | GLU  |
| 1   | B     | 82   | THR  |
| 1   | B     | 95   | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 111 | VAL  |
| 1   | B     | 121 | LEU  |
| 1   | B     | 134 | ARG  |
| 1   | B     | 141 | LEU  |
| 1   | B     | 152 | MET  |
| 1   | B     | 154 | LEU  |
| 1   | B     | 175 | ARG  |
| 1   | B     | 180 | ILE  |
| 1   | B     | 184 | GLU  |
| 1   | B     | 194 | LEU  |
| 1   | B     | 198 | LYS  |
| 1   | B     | 204 | ARG  |
| 1   | B     | 206 | LYS  |
| 1   | B     | 211 | GLU  |
| 1   | B     | 213 | PRO  |
| 1   | B     | 215 | VAL  |
| 1   | B     | 218 | THR  |
| 1   | B     | 227 | GLN  |
| 1   | B     | 248 | GLN  |
| 1   | B     | 257 | SER  |
| 1   | B     | 260 | LEU  |
| 1   | B     | 273 | ILE  |
| 1   | B     | 279 | SER  |
| 1   | B     | 287 | ILE  |
| 1   | B     | 290 | LEU  |
| 1   | B     | 302 | VAL  |
| 1   | B     | 303 | ARG  |
| 1   | B     | 317 | LEU  |
| 1   | B     | 324 | ILE  |
| 1   | B     | 325 | THR  |
| 1   | B     | 328 | ASP  |
| 1   | B     | 331 | LYS  |
| 1   | B     | 342 | LEU  |
| 1   | B     | 349 | VAL  |
| 1   | B     | 351 | ARG  |
| 1   | B     | 357 | LYS  |
| 1   | B     | 359 | LEU  |
| 1   | B     | 365 | LEU  |
| 1   | B     | 367 | SER  |
| 1   | B     | 392 | VAL  |
| 1   | B     | 398 | VAL  |
| 1   | B     | 399 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 403 | LEU  |
| 1   | B     | 415 | LYS  |
| 1   | B     | 439 | LYS  |
| 1   | B     | 454 | SER  |
| 1   | B     | 460 | SER  |
| 1   | B     | 463 | ILE  |
| 1   | B     | 465 | ILE  |
| 1   | B     | 468 | LEU  |
| 1   | B     | 472 | GLU  |
| 1   | B     | 482 | ASN  |
| 1   | B     | 501 | LEU  |
| 1   | B     | 509 | THR  |
| 1   | B     | 511 | VAL  |
| 1   | B     | 512 | LEU  |
| 1   | B     | 514 | SER  |
| 1   | B     | 517 | SER  |
| 1   | B     | 532 | ARG  |
| 1   | B     | 538 | LYS  |
| 1   | B     | 570 | LEU  |
| 1   | B     | 582 | LEU  |
| 1   | B     | 583 | LEU  |
| 1   | B     | 593 | LYS  |
| 1   | B     | 613 | LEU  |
| 1   | B     | 617 | LYS  |
| 1   | B     | 621 | SER  |
| 1   | B     | 628 | GLU  |
| 1   | B     | 629 | THR  |
| 1   | B     | 630 | LYS  |
| 1   | B     | 635 | THR  |
| 1   | B     | 637 | GLU  |
| 1   | B     | 643 | VAL  |
| 1   | B     | 654 | LEU  |
| 1   | B     | 656 | VAL  |
| 1   | B     | 673 | GLU  |
| 1   | B     | 677 | VAL  |
| 1   | B     | 681 | VAL  |
| 1   | B     | 683 | GLN  |
| 1   | B     | 687 | GLU  |
| 1   | B     | 698 | VAL  |
| 1   | B     | 702 | SER  |
| 1   | B     | 710 | LYS  |
| 1   | B     | 714 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 715  | VAL  |
| 1   | B     | 718  | PRO  |
| 1   | B     | 720  | ASN  |
| 1   | B     | 725  | GLU  |
| 1   | B     | 730  | GLU  |
| 1   | B     | 737  | ARG  |
| 1   | B     | 741  | ASN  |
| 1   | B     | 771  | ARG  |
| 1   | B     | 778  | LEU  |
| 1   | B     | 783  | ARG  |
| 1   | B     | 800  | GLN  |
| 1   | B     | 808  | PHE  |
| 1   | B     | 821  | VAL  |
| 1   | B     | 823  | VAL  |
| 1   | B     | 851  | MET  |
| 1   | B     | 854  | LYS  |
| 1   | B     | 857  | ARG  |
| 1   | B     | 858  | LEU  |
| 1   | B     | 874  | GLU  |
| 1   | B     | 883  | MET  |
| 1   | B     | 887  | ARG  |
| 1   | B     | 910  | LEU  |
| 1   | B     | 914  | LEU  |
| 1   | B     | 917  | LYS  |
| 1   | B     | 921  | ILE  |
| 1   | B     | 930  | LEU  |
| 1   | B     | 941  | LEU  |
| 1   | B     | 942  | LEU  |
| 1   | B     | 949  | SER  |
| 1   | B     | 953  | THR  |
| 1   | B     | 954  | LYS  |
| 1   | B     | 955  | LYS  |
| 1   | B     | 986  | VAL  |
| 1   | B     | 997  | THR  |
| 1   | B     | 1001 | SER  |
| 1   | B     | 1002 | SER  |
| 1   | B     | 1029 | VAL  |
| 1   | B     | 1048 | GLN  |
| 1   | B     | 1064 | LEU  |
| 1   | B     | 1074 | GLN  |
| 1   | B     | 1104 | ARG  |
| 1   | B     | 1105 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1108 | GLN  |
| 1   | B     | 1110 | LYS  |
| 1   | B     | 1118 | LYS  |
| 1   | B     | 1124 | VAL  |
| 1   | B     | 1126 | GLU  |
| 1   | B     | 1136 | VAL  |
| 1   | B     | 1137 | LEU  |
| 1   | B     | 1146 | LYS  |
| 1   | B     | 1149 | ARG  |
| 1   | B     | 1166 | MET  |
| 1   | B     | 1170 | ASN  |
| 1   | B     | 1171 | ILE  |
| 1   | B     | 1173 | GLU  |
| 1   | B     | 1181 | LYS  |
| 1   | B     | 1185 | SER  |
| 1   | B     | 1186 | VAL  |
| 1   | B     | 1196 | THR  |
| 1   | B     | 1197 | ARG  |
| 1   | B     | 1199 | ASP  |
| 1   | B     | 1200 | THR  |
| 1   | B     | 1205 | ARG  |
| 1   | B     | 1219 | THR  |
| 1   | B     | 1223 | GLN  |
| 1   | B     | 1225 | ASP  |
| 1   | B     | 1232 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) 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     | 147 | GLN  |
| 1   | A     | 169 | HIS  |
| 1   | A     | 212 | HIS  |
| 1   | A     | 220 | GLN  |
| 1   | A     | 227 | GLN  |
| 1   | A     | 233 | ASN  |
| 1   | A     | 288 | ASN  |
| 1   | A     | 389 | HIS  |
| 1   | A     | 421 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 434  | ASN  |
| 1   | A     | 467  | HIS  |
| 1   | A     | 491  | ASN  |
| 1   | A     | 536  | ASN  |
| 1   | A     | 543  | ASN  |
| 1   | A     | 560  | ASN  |
| 1   | A     | 636  | ASN  |
| 1   | A     | 650  | GLN  |
| 1   | A     | 688  | ASN  |
| 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     | 777  | ASN  |
| 1   | A     | 800  | GLN  |
| 1   | A     | 918  | ASN  |
| 1   | A     | 976  | HIS  |
| 1   | A     | 996  | ASN  |
| 1   | A     | 1000 | GLN  |
| 1   | A     | 1047 | GLN  |
| 1   | A     | 1048 | GLN  |
| 1   | A     | 1088 | ASN  |
| 1   | A     | 1108 | GLN  |
| 1   | A     | 1111 | ASN  |
| 1   | A     | 1132 | ASN  |
| 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     | 147  | GLN  |
| 1   | B     | 169  | HIS  |
| 1   | B     | 212  | HIS  |
| 1   | B     | 220  | GLN  |
| 1   | B     | 227  | GLN  |
| 1   | B     | 233  | ASN  |
| 1   | B     | 288  | ASN  |
| 1   | B     | 389  | HIS  |
| 1   | B     | 421  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 434  | ASN  |
| 1   | B     | 467  | HIS  |
| 1   | B     | 491  | ASN  |
| 1   | B     | 536  | ASN  |
| 1   | B     | 543  | ASN  |
| 1   | B     | 560  | ASN  |
| 1   | B     | 636  | ASN  |
| 1   | B     | 650  | GLN  |
| 1   | B     | 688  | ASN  |
| 1   | B     | 693  | ASN  |
| 1   | B     | 720  | ASN  |
| 1   | B     | 739  | GLN  |
| 1   | B     | 741  | ASN  |
| 1   | B     | 750  | ASN  |
| 1   | B     | 777  | ASN  |
| 1   | B     | 800  | GLN  |
| 1   | B     | 918  | ASN  |
| 1   | B     | 976  | HIS  |
| 1   | B     | 996  | ASN  |
| 1   | B     | 1000 | GLN  |
| 1   | B     | 1047 | GLN  |
| 1   | B     | 1048 | GLN  |
| 1   | B     | 1088 | ASN  |
| 1   | B     | 1108 | GLN  |
| 1   | B     | 1111 | ASN  |
| 1   | B     | 1132 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

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  | B     | 1242 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 5   | TPP  | A     | 1236 | 2    | 26,27,27     | 1.42 | 5 (19%)  | 38,40,40    | 1.89 | 8 (21%)  |
| 5   | TPP  | B     | 1243 | 2    | 26,27,27     | 1.42 | 5 (19%)  | 38,40,40    | 1.89 | 8 (21%)  |
| 4   | SF4  | A     | 1235 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 4   | SF4  | A     | 1233 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 4   | SF4  | B     | 1240 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 6   | PYR  | B     | 1246 | -    | 5,5,5        | 4.14 | 3 (60%)  | 3,6,6       | 2.84 | 2 (66%)  |
| 4   | SF4  | B     | 1241 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 4   | SF4  | A     | 1234 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 6   | PYR  | A     | 1239 | -    | 5,5,5        | 4.15 | 3 (60%)  | 3,6,6       | 2.83 | 2 (66%)  |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 5   | TPP  | A     | 1236 | 2    | -       | 9/17/17/17 | 0/2/2/2 |
| 4   | SF4  | B     | 1242 | 1    | -       | -          | 0/6/5/5 |
| 5   | TPP  | B     | 1243 | 2    | -       | 9/17/17/17 | 0/2/2/2 |
| 4   | SF4  | A     | 1235 | 1    | -       | -          | 0/6/5/5 |
| 4   | SF4  | A     | 1233 | 1    | -       | -          | 0/6/5/5 |
| 4   | SF4  | B     | 1240 | 1    | -       | -          | 0/6/5/5 |
| 6   | PYR  | B     | 1246 | -    | -       | 0/4/4/4    | -       |
| 4   | SF4  | B     | 1241 | 1    | -       | -          | 0/6/5/5 |
| 4   | SF4  | A     | 1234 | 1    | -       | -          | 0/6/5/5 |
| 6   | PYR  | A     | 1239 | -    | -       | 0/4/4/4    | -       |

All (16) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 6   | A     | 1239 | PYR  | O3-CA   | 7.81  | 1.41        | 1.23     |
| 6   | B     | 1246 | PYR  | O3-CA   | 7.79  | 1.40        | 1.23     |
| 6   | A     | 1239 | PYR  | CA-C    | -3.51 | 1.42        | 1.54     |
| 6   | B     | 1246 | PYR  | CA-C    | -3.49 | 1.42        | 1.54     |
| 6   | B     | 1246 | PYR  | O-C     | 3.38  | 1.30        | 1.22     |
| 6   | A     | 1239 | PYR  | O-C     | 3.38  | 1.30        | 1.22     |
| 5   | B     | 1243 | TPP  | C4'-N3' | 3.20  | 1.39        | 1.35     |
| 5   | A     | 1236 | TPP  | C4'-N3' | 3.16  | 1.39        | 1.35     |
| 5   | A     | 1236 | TPP  | C2'-N1' | 3.00  | 1.38        | 1.34     |
| 5   | B     | 1243 | TPP  | C2'-N1' | 2.98  | 1.38        | 1.34     |
| 5   | B     | 1243 | TPP  | PB-O3B  | -2.44 | 1.45        | 1.54     |
| 5   | A     | 1236 | TPP  | PB-O3B  | -2.44 | 1.45        | 1.54     |
| 5   | A     | 1236 | TPP  | C7'-N3  | 2.38  | 1.53        | 1.48     |
| 5   | B     | 1243 | TPP  | C7'-N3  | 2.38  | 1.53        | 1.48     |
| 5   | B     | 1243 | TPP  | PA-O3A  | -2.17 | 1.57        | 1.59     |
| 5   | A     | 1236 | TPP  | PA-O3A  | -2.14 | 1.57        | 1.59     |

All (20) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | A     | 1236 | TPP  | C7'-N3-C2   | 6.12  | 136.25      | 123.48   |
| 5   | B     | 1243 | TPP  | C7'-N3-C2   | 6.11  | 136.24      | 123.48   |
| 5   | B     | 1243 | TPP  | O3B-PB-O2B  | 3.80  | 122.06      | 107.80   |
| 5   | A     | 1236 | TPP  | O3B-PB-O2B  | 3.80  | 122.04      | 107.80   |
| 5   | B     | 1243 | TPP  | C2-N3-C4    | -3.72 | 109.03      | 114.06   |
| 5   | A     | 1236 | TPP  | C2-N3-C4    | -3.72 | 109.03      | 114.06   |
| 5   | A     | 1236 | TPP  | CM2-C2'-N1' | 3.64  | 121.08      | 117.20   |
| 5   | B     | 1243 | TPP  | CM2-C2'-N1' | 3.63  | 121.07      | 117.20   |
| 6   | B     | 1246 | PYR  | OXT-C-CA    | 3.46  | 123.19      | 113.59   |
| 6   | A     | 1239 | PYR  | OXT-C-CA    | 3.45  | 123.16      | 113.59   |
| 6   | B     | 1246 | PYR  | OXT-C-O     | -3.43 | 115.74      | 123.90   |
| 6   | A     | 1239 | PYR  | OXT-C-O     | -3.42 | 115.75      | 123.90   |
| 5   | A     | 1236 | TPP  | C7'-N3-C4   | -3.15 | 114.01      | 122.36   |
| 5   | B     | 1243 | TPP  | C7'-N3-C4   | -3.15 | 114.02      | 122.36   |
| 5   | A     | 1236 | TPP  | N1'-C2'-N3' | -2.50 | 121.37      | 125.53   |
| 5   | B     | 1243 | TPP  | N1'-C2'-N3' | -2.48 | 121.40      | 125.53   |
| 5   | A     | 1236 | TPP  | PA-O7-C7    | 2.41  | 132.75      | 121.26   |
| 5   | B     | 1243 | TPP  | PA-O7-C7    | 2.41  | 132.75      | 121.26   |
| 5   | A     | 1236 | TPP  | C2-S1-C5    | -2.21 | 89.75       | 91.22    |
| 5   | B     | 1243 | TPP  | C2-S1-C5    | -2.21 | 89.75       | 91.22    |

There are no chirality outliers.

All (18) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 5   | A     | 1236 | TPP  | C7-O7-PA-O2A   |
| 5   | A     | 1236 | TPP  | C7-O7-PA-O3A   |
| 5   | A     | 1236 | TPP  | PA-O3A-PB-O3B  |
| 5   | B     | 1243 | TPP  | C7-O7-PA-O2A   |
| 5   | B     | 1243 | TPP  | C7-O7-PA-O3A   |
| 5   | B     | 1243 | TPP  | PA-O3A-PB-O3B  |
| 5   | A     | 1236 | TPP  | C5'-C7'-N3-C2  |
| 5   | B     | 1243 | TPP  | C5'-C7'-N3-C2  |
| 5   | A     | 1236 | TPP  | C5-C6-C7-O7    |
| 5   | B     | 1243 | TPP  | C5-C6-C7-O7    |
| 5   | A     | 1236 | TPP  | C7-O7-PA-O1A   |
| 5   | B     | 1243 | TPP  | C7-O7-PA-O1A   |
| 5   | A     | 1236 | TPP  | PB-O3A-PA-O2A  |
| 5   | B     | 1243 | TPP  | PB-O3A-PA-O2A  |
| 5   | A     | 1236 | TPP  | C4'-C5'-C7'-N3 |
| 5   | B     | 1243 | TPP  | C4'-C5'-C7'-N3 |
| 5   | A     | 1236 | TPP  | PB-O3A-PA-O1A  |
| 5   | B     | 1243 | TPP  | PB-O3A-PA-O1A  |

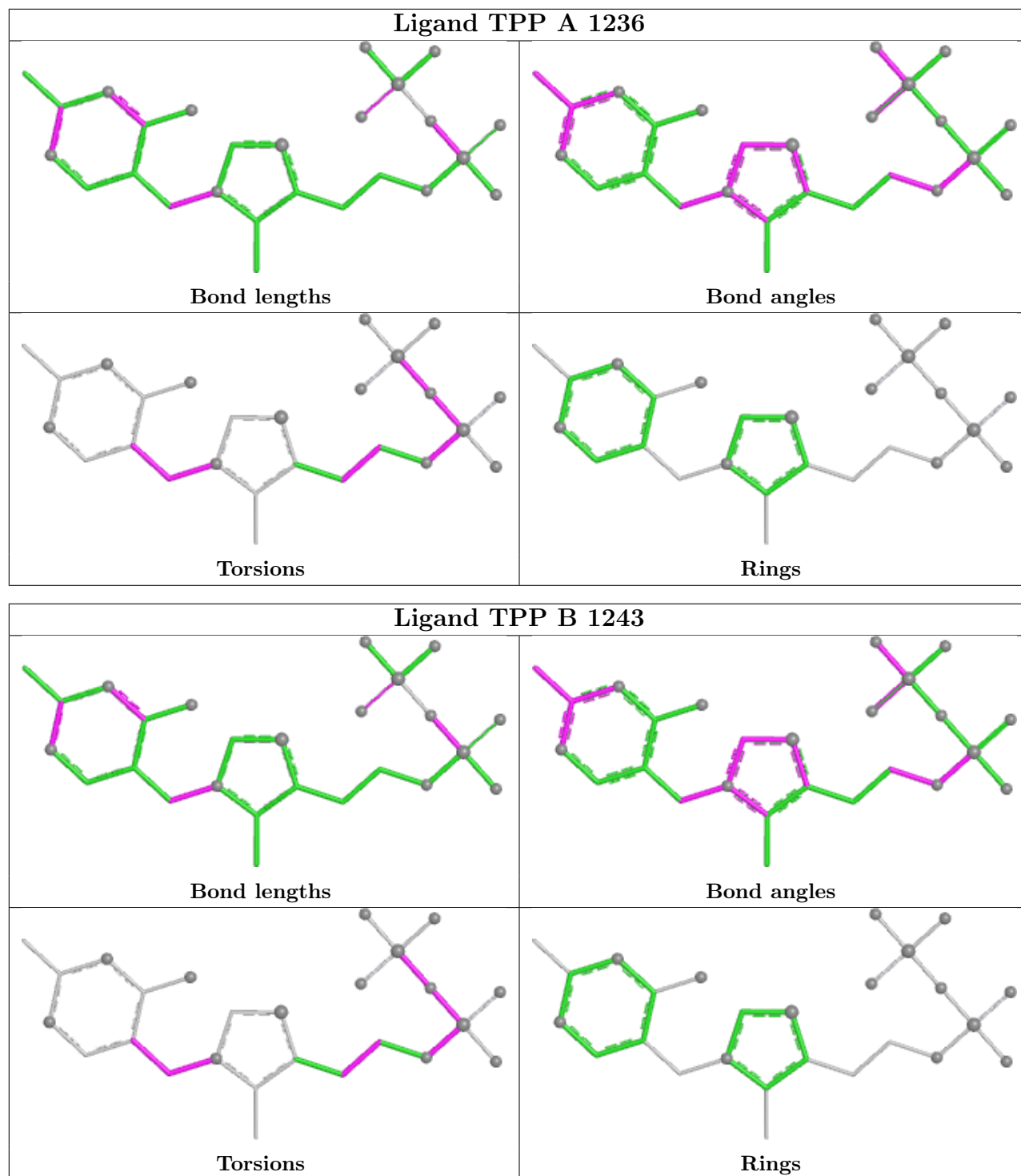
There are no ring outliers.

10 monomers are involved in 20 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | B     | 1242 | SF4  | 1       | 0            |
| 5   | A     | 1236 | TPP  | 6       | 0            |
| 5   | B     | 1243 | TPP  | 6       | 0            |
| 4   | A     | 1235 | SF4  | 1       | 0            |
| 4   | A     | 1233 | SF4  | 1       | 0            |
| 4   | B     | 1240 | SF4  | 1       | 0            |
| 6   | B     | 1246 | PYR  | 2       | 0            |
| 4   | B     | 1241 | SF4  | 2       | 0            |
| 4   | A     | 1234 | SF4  | 2       | 0            |
| 6   | A     | 1239 | PYR  | 2       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.