



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:17 PM UTC

PDB ID : 7FJJ / pdb\_00007fjj  
EMDB ID : EMD-31622  
Title : human Pol III pre-termination complex  
Authors : Hou, H.; Xu, Y.  
Deposited on : 2021-08-04  
Resolution : 3.60 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

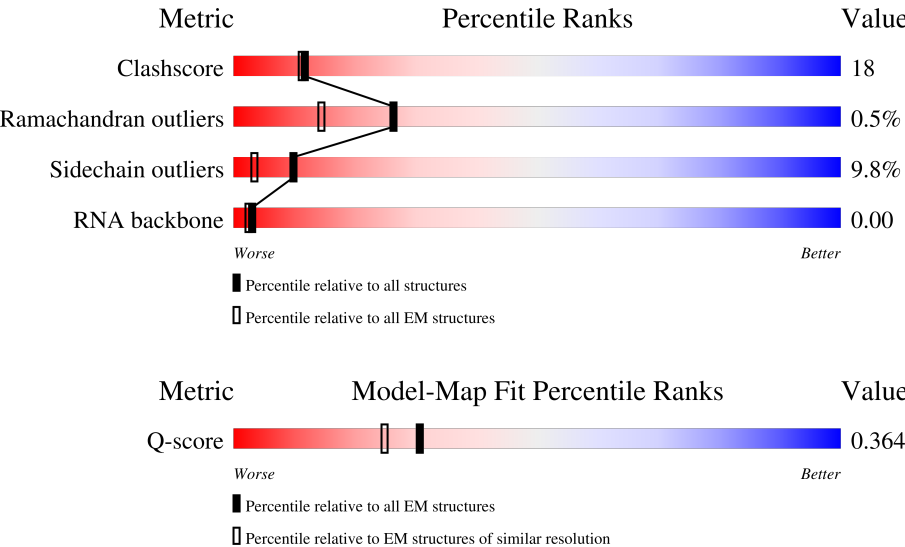
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

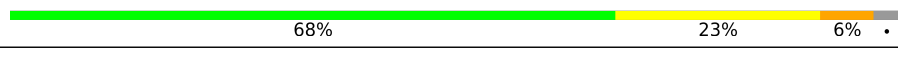
The reported resolution of this entry is 3.60 Å.

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.



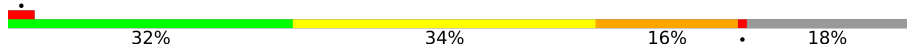
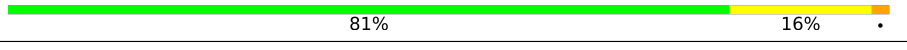
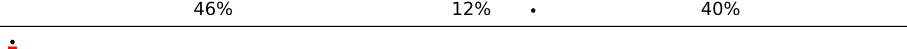
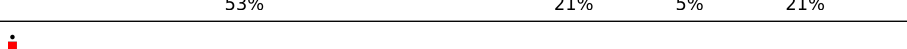
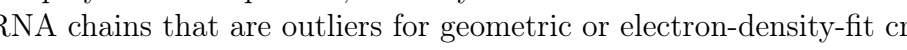
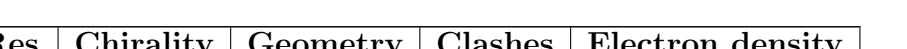
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 12797 ( 3.10 - 4.10 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 1390   |  |
| 2   | B     | 1133   |  |
| 3   | C     | 346    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | D     | 148    |    |
| 5   | E     | 210    |    |
| 6   | F     | 127    |    |
| 7   | G     | 204    |    |
| 8   | H     | 150    |    |
| 9   | I     | 108    |    |
| 10  | J     | 67     |    |
| 11  | K     | 133    |    |
| 12  | L     | 58     |    |
| 13  | M     | 708    |   |
| 14  | N     | 398    |  |
| 15  | O     | 534    |  |
| 16  | P     | 316    |  |
| 17  | Q     | 223    |  |
| 18  | R     | 10     |  |
| 19  | X     | 54     |  |
| 20  | Y     | 54     |  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 22  | ZN   | J     | 2000 | -         | -        | X       | -                |
| 23  | SF4  | P     | 401  | -         | -        | X       | -                |

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 39474 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 DNA-directed RNA polymerase III subunit RPC1.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 1360     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10675 | 6763 | 1865 | 1974 | 73 |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | B     | 1095     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8644  | 5473 | 1512 | 1591 | 68 |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 343      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2736  | 1723 | 488 | 514 | 11 |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 985   | 614 | 172 | 196 | 3 |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | E     | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1715  | 1083 | 300 | 324 | 8 |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 76       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 610   | 392 | 103 | 110 | 5 |         |       |

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G     | 166      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1337  | 876 | 211 | 245 | 5 |         |       |

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1186  | 750 | 194 | 237 | 5 |         |       |

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 9   | I     | 107      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 848   | 525 | 157 | 153 | 13 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| I     | 24      | ALA      | SER    | variant | UNP Q9Y2Y1 |

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10  | J     | 65       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 512   | 331 | 87 | 88 | 6 |         |       |

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | K     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 822   | 513 | 145 | 157 | 7 |         |       |

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 12  | L     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 388   | 241 | 75 | 66 | 6 |         |       |

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13  | M     | 202      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1612  | 1012 | 274 | 316 | 10 |         |       |

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | N     | 146      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1128  | 710 | 191 | 221 | 6 |         |       |

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | O     | 443      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3546  | 2233 | 620 | 673 | 20 |         |       |

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 16  | P     | 130      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1008  | 636 | 166 | 196 | 10 |         |       |

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | Q     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 724   | 463 | 124 | 131 | 6 |         |       |

- Molecule 18 is a RNA chain called RNA (5'-R(\*CP\*CP\*GP\*GP\*GP\*UP\*GP\*CP\*UP\*G)-3').

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 18  | R     | 4        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 86    | 38 | 15 | 29 | 4 |         |       |

- Molecule 19 is a DNA chain called non-template DNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 19  | X     | 22       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 449   | 215 | 76 | 136 | 22 |         |       |

- Molecule 20 is a DNA chain called template DNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 20  | Y     | 22       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 447   | 212 | 79 | 134 | 22 |         |       |

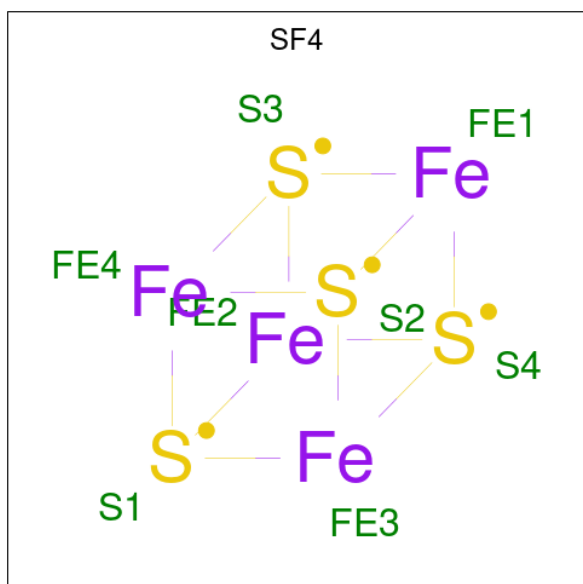
- Molecule 21 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 21  | A     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 22  | A     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 22  | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 22  | I     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 22  | J     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 22  | L     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).

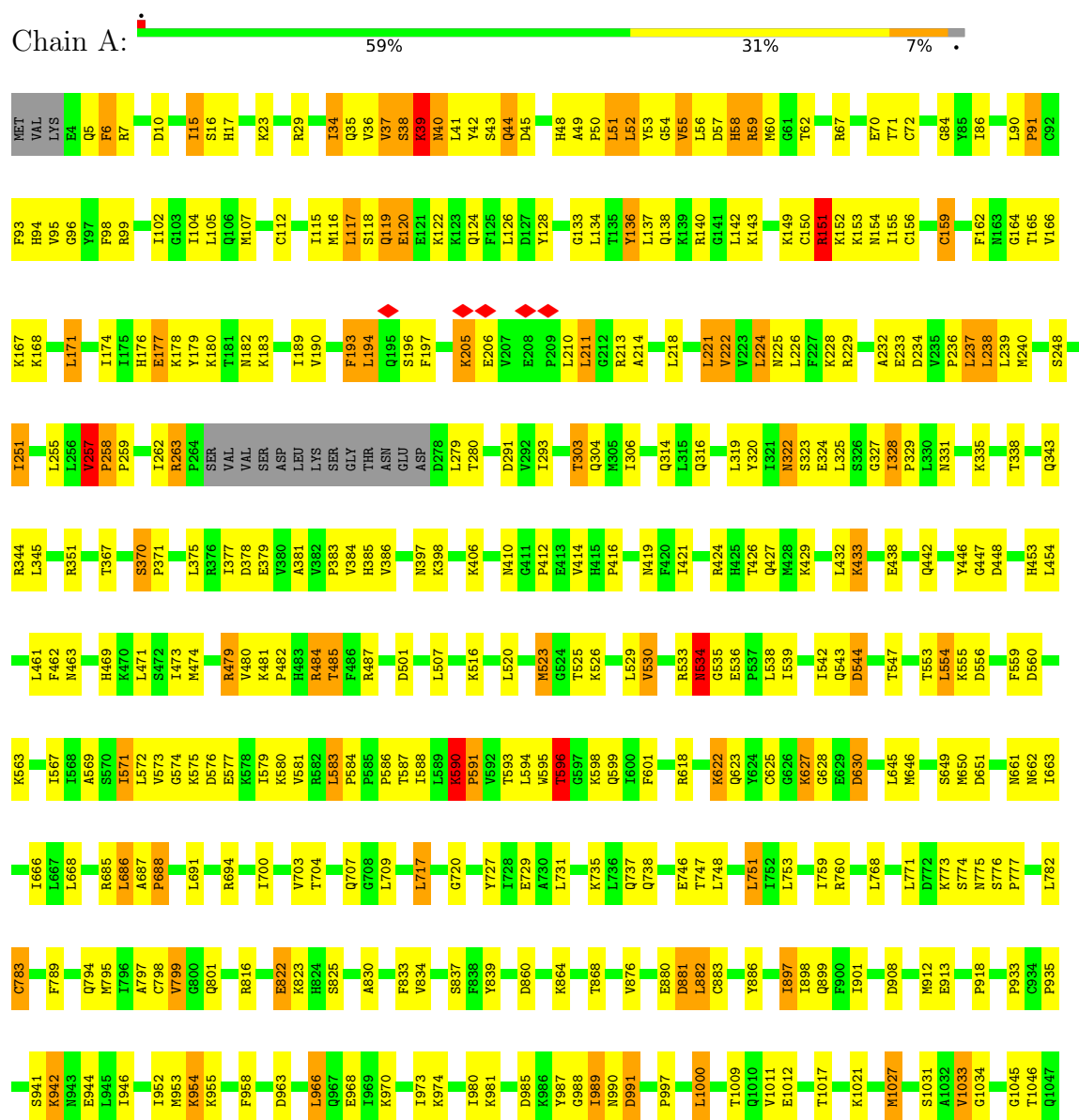


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
|     |       |          | Total | Fe | S |         |
| 23  | P     | 1        | 8     | 4  | 4 | 0       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase III subunit RPC1

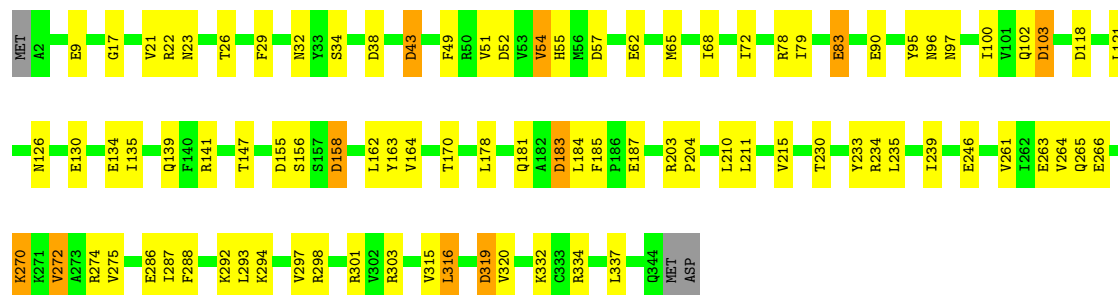






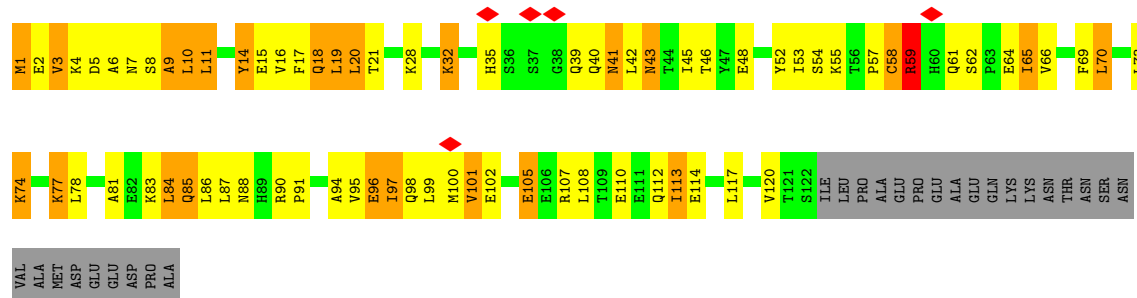
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 73% 23%



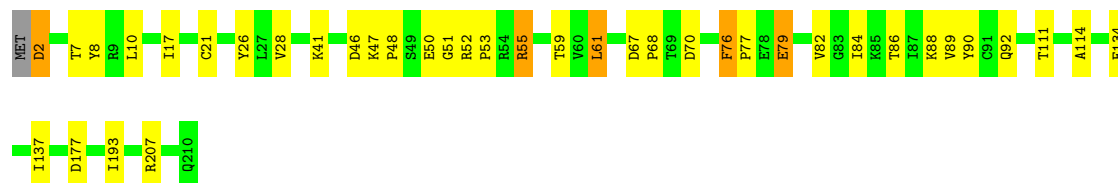
- Molecule 4: DNA-directed RNA polymerase III subunit RPC9

Chain D: 32% 34% 16% 18%



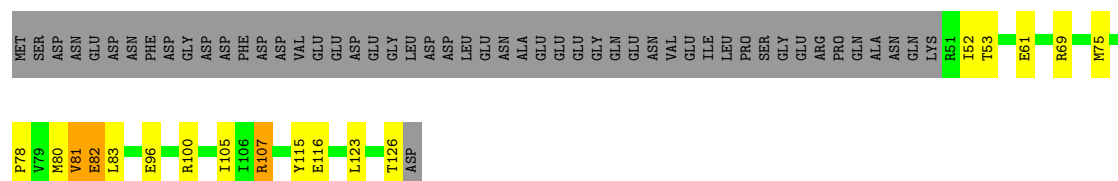
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 81% 16%

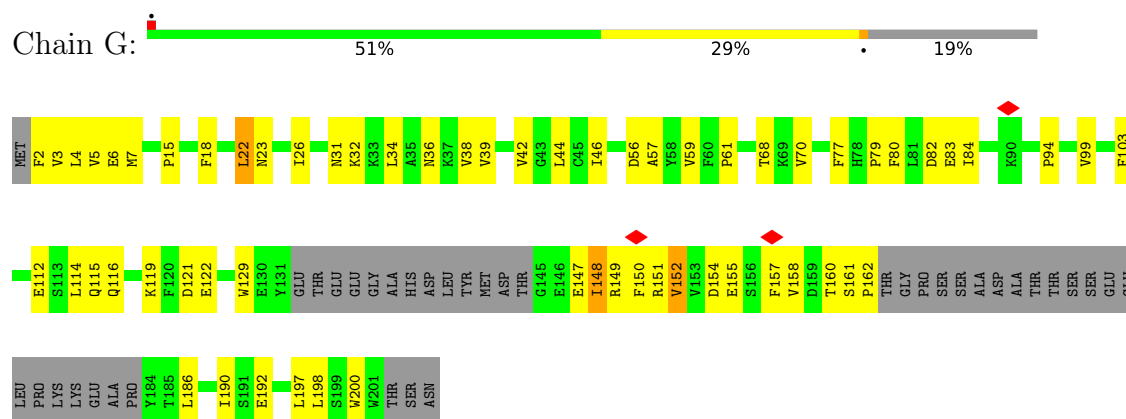


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

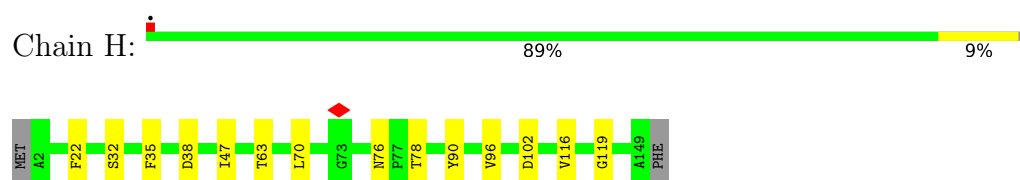
Chain F: 46% 12% 40%



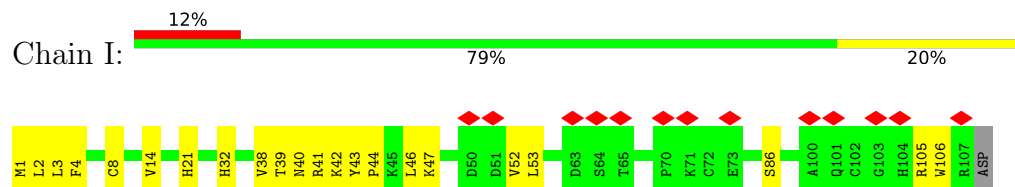
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8



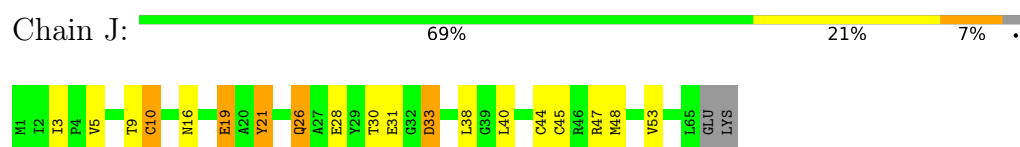
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



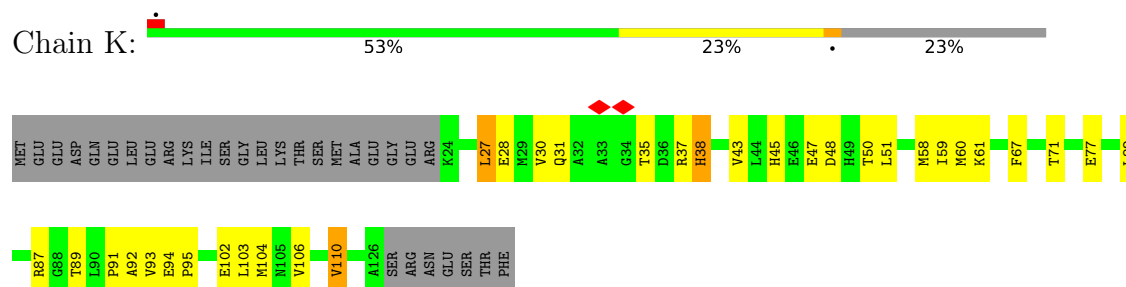
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

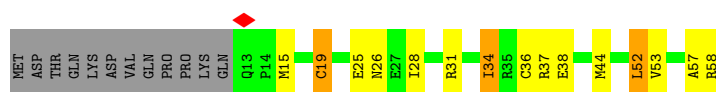


- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

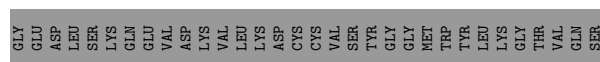
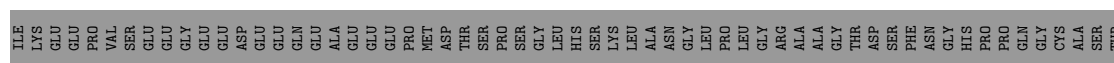
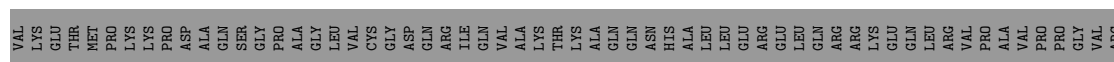
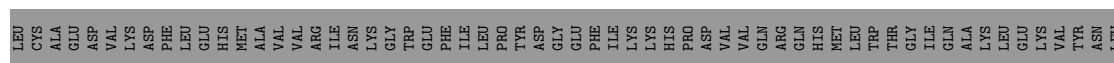
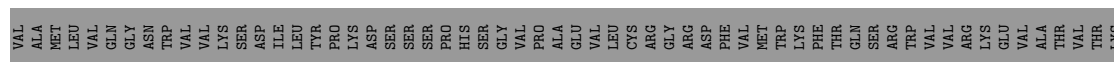
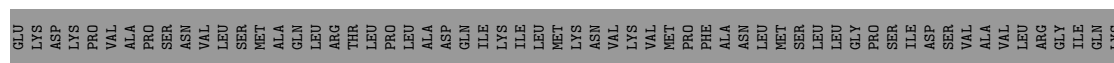


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



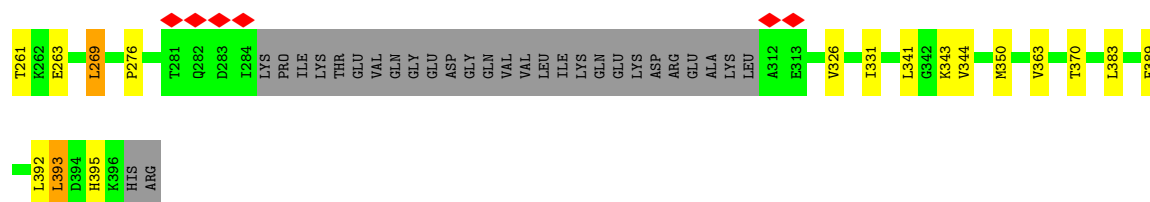


• Molecule 13: DNA-directed RNA polymerase III subunit RPC5

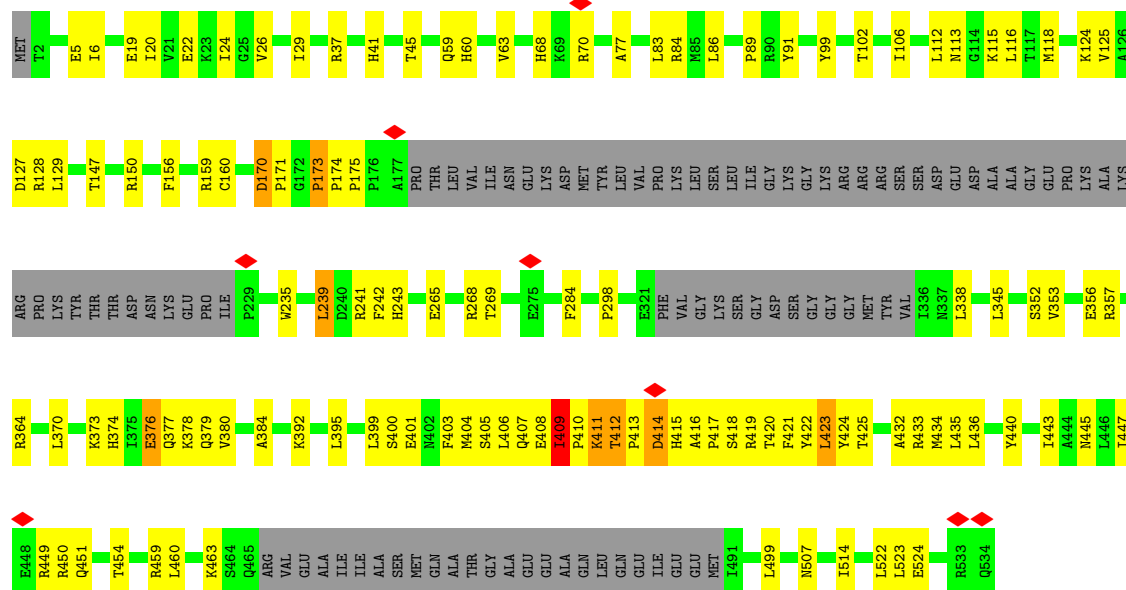


• Molecule 14: DNA-directed RNA polymerase III subunit RPC4

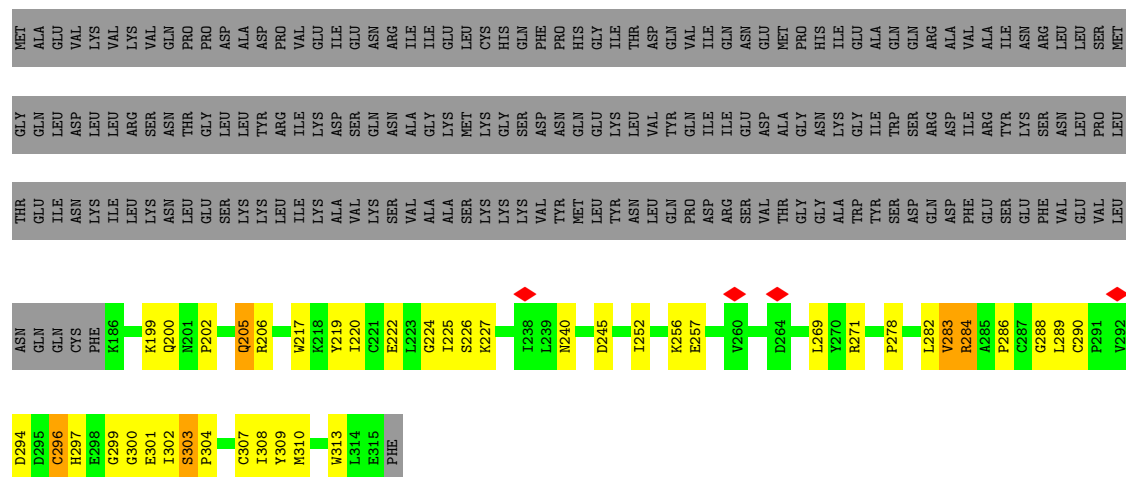




• Molecule 15: DNA-directed RNA polymerase III subunit RPC3

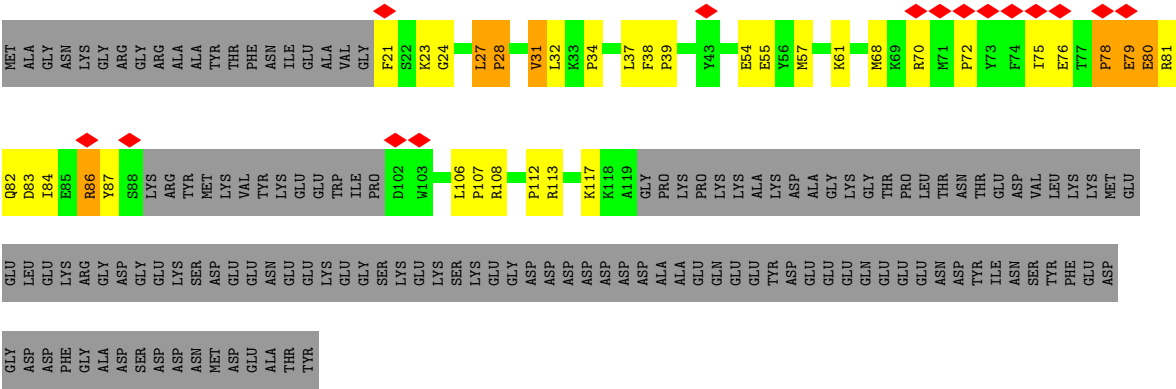


• Molecule 16: DNA-directed RNA polymerase III subunit RPC6



• Molecule 17: DNA-directed RNA polymerase III subunit RPC7

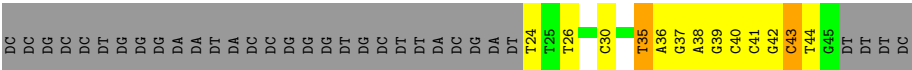




● Molecule 18: RNA (5'-R(\*CP\*CP\*GP\*GP\*GP\*UP\*GP\*CP\*UP\*G)-3')



● Molecule 19: non-template DNA



● Molecule 20: template DNA



## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, Not provided       |           |
| Number of particles used             | 48593                     | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF         | Depositor |
| CTF correction method                | NONE                      | Depositor |
| Microscope                           | FEI TITAN KRIOS           | Depositor |
| Voltage (kV)                         | 300                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1.38                      | Depositor |
| Minimum defocus (nm)                 | Not provided              |           |
| Maximum defocus (nm)                 | Not provided              |           |
| Magnification                        | Not provided              |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value                    | 0.080                     | Depositor |
| Minimum map value                    | -0.024                    | Depositor |
| Average map value                    | 0.000                     | Depositor |
| Map value standard deviation         | 0.002                     | Depositor |
| Recommended contour level            | 0.006                     | Depositor |
| Map size ( $\text{\AA}$ )            | 379.44, 379.44, 379.44    | wwPDB     |
| Map dimensions                       | 360, 360, 360             | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0          | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.054, 1.054, 1.054       | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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     | 0.95         | 6/10866 (0.1%) | 1.35        | 39/14648 (0.3%)  |
| 2   | B     | 0.95         | 1/8807 (0.0%)  | 1.33        | 28/11875 (0.2%)  |
| 3   | C     | 0.90         | 0/2790         | 1.20        | 3/3782 (0.1%)    |
| 4   | D     | 0.86         | 0/997          | 1.42        | 6/1343 (0.4%)    |
| 5   | E     | 0.59         | 0/1745         | 0.95        | 4/2358 (0.2%)    |
| 6   | F     | 0.89         | 0/620          | 1.20        | 0/839            |
| 7   | G     | 0.54         | 0/1374         | 0.97        | 3/1868 (0.2%)    |
| 8   | H     | 0.33         | 0/1207         | 0.63        | 0/1628           |
| 9   | I     | 0.27         | 0/869          | 0.63        | 0/1174           |
| 10  | J     | 0.85         | 0/521          | 1.30        | 1/703 (0.1%)     |
| 11  | K     | 0.84         | 0/837          | 1.24        | 1/1129 (0.1%)    |
| 12  | L     | 0.87         | 0/394          | 1.14        | 0/524            |
| 13  | M     | 0.72         | 0/1648         | 0.88        | 0/2232           |
| 14  | N     | 0.77         | 0/1137         | 0.97        | 2/1530 (0.1%)    |
| 15  | O     | 0.42         | 0/3604         | 0.75        | 5/4872 (0.1%)    |
| 16  | P     | 0.54         | 0/1028         | 0.95        | 2/1391 (0.1%)    |
| 17  | Q     | 0.61         | 0/742          | 0.93        | 1/996 (0.1%)     |
| 18  | R     | 0.73         | 0/95           | 0.95        | 0/146            |
| 19  | X     | 0.45         | 0/501          | 0.96        | 2/771 (0.3%)     |
| 20  | Y     | 0.47         | 0/499          | 1.19        | 5/767 (0.7%)     |
| All | All   | 0.82         | 7/40281 (0.0%) | 1.18        | 102/54576 (0.2%) |

All (7) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | B     | 1082 | GLN  | C-N   | -7.88 | 1.23        | 1.33     |
| 1   | A     | 258  | PRO  | C-O   | -6.11 | 1.19        | 1.25     |
| 1   | A     | 694  | ARG  | C-O   | -5.72 | 1.17        | 1.24     |
| 1   | A     | 559  | PHE  | C-O   | -5.68 | 1.17        | 1.23     |
| 1   | A     | 91   | PRO  | C-O   | -5.24 | 1.17        | 1.23     |
| 1   | A     | 584  | PRO  | C-O   | -5.24 | 1.20        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 688 | PRO  | C-O   | -5.11 | 1.17        | 1.24     |

All (102) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 2   | B     | 1083 | CYS  | CB-CA-C     | 17.40  | 137.92      | 110.95   |
| 2   | B     | 1083 | CYS  | N-CA-CB     | -11.68 | 93.05       | 109.98   |
| 2   | B     | 1095 | CYS  | N-CA-C      | -11.11 | 84.97       | 107.41   |
| 1   | A     | 37   | VAL  | N-CA-C      | -9.90  | 102.99      | 112.29   |
| 1   | A     | 40   | ASN  | N-CA-C      | -9.36  | 101.78      | 113.01   |
| 20  | Y     | 1    | DG   | C2'-C3'-O3' | -9.30  | 97.55       | 111.50   |
| 2   | B     | 1095 | CYS  | N-CA-CB     | -8.80  | 94.19       | 110.56   |
| 2   | B     | 1042 | ASP  | CB-CA-C     | 8.52   | 118.27      | 109.83   |
| 2   | B     | 1084 | GLY  | N-CA-C      | -8.26  | 103.32      | 115.63   |
| 2   | B     | 1082 | GLN  | CA-C-N      | 7.92   | 131.40      | 120.63   |
| 2   | B     | 1082 | GLN  | C-N-CA      | 7.92   | 131.40      | 120.63   |
| 1   | A     | 258  | PRO  | N-CA-CB     | -7.81  | 98.82       | 103.19   |
| 1   | A     | 59   | ARG  | N-CA-C      | -7.76  | 103.95      | 113.50   |
| 1   | A     | 238  | LEU  | N-CA-C      | -7.54  | 103.81      | 113.16   |
| 4   | D     | 58   | CYS  | N-CA-C      | -7.42  | 103.97      | 112.87   |
| 15  | O     | 412  | THR  | CB-CA-C     | 7.39   | 120.19      | 109.11   |
| 20  | Y     | 0    | DA   | C2'-C3'-O3' | -7.32  | 100.52      | 111.50   |
| 2   | B     | 1122 | ILE  | CA-C-N      | -7.25  | 117.67      | 122.60   |
| 2   | B     | 1122 | ILE  | C-N-CA      | -7.25  | 117.67      | 122.60   |
| 4   | D     | 10   | LEU  | N-CA-C      | -7.16  | 101.87      | 113.19   |
| 20  | Y     | 5    | DC   | C2'-C3'-O3' | -7.13  | 100.80      | 111.50   |
| 7   | G     | 148  | ILE  | CA-C-N      | -6.91  | 113.30      | 123.11   |
| 7   | G     | 148  | ILE  | C-N-CA      | -6.91  | 113.30      | 123.11   |
| 20  | Y     | 4    | DG   | C2'-C3'-O3' | -6.83  | 101.26      | 111.50   |
| 1   | A     | 591  | PRO  | N-CA-C      | -6.82  | 103.72      | 113.47   |
| 7   | G     | 158  | VAL  | N-CA-C      | 6.78   | 117.56      | 110.72   |
| 1   | A     | 830  | ALA  | N-CA-C      | -6.71  | 105.13      | 113.38   |
| 1   | A     | 44   | GLN  | N-CA-C      | -6.71  | 99.90       | 109.96   |
| 19  | X     | 43   | DC   | C2'-C3'-O3' | 6.58   | 121.37      | 111.50   |
| 10  | J     | 10   | CYS  | CB-CA-C     | 6.48   | 121.86      | 110.85   |
| 1   | A     | 746  | GLU  | N-CA-C      | -6.46  | 105.29      | 113.43   |
| 1   | A     | 258  | PRO  | N-CA-C      | 6.45   | 116.67      | 110.47   |
| 1   | A     | 918  | PRO  | N-CA-C      | 6.43   | 122.47      | 113.53   |
| 1   | A     | 933  | PRO  | N-CA-C      | -6.29  | 99.51       | 112.47   |
| 1   | A     | 622  | LYS  | CA-C-O      | -6.11  | 114.90      | 121.56   |
| 1   | A     | 1049 | THR  | N-CA-C      | -6.10  | 105.60      | 113.16   |
| 15  | O     | 173  | PRO  | N-CA-C      | 6.07   | 118.11      | 110.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | B     | 817  | PRO  | N-CA-CB     | -6.05 | 97.74       | 103.19   |
| 1   | A     | 167  | LYS  | N-CA-C      | 6.04  | 119.89      | 111.56   |
| 2   | B     | 380  | PHE  | CA-CB-CG    | 5.99  | 119.79      | 113.80   |
| 1   | A     | 783  | CYS  | N-CA-C      | -5.88 | 101.24      | 110.36   |
| 2   | B     | 514  | LEU  | N-CA-C      | -5.88 | 104.88      | 111.28   |
| 1   | A     | 935  | PRO  | N-CA-C      | -5.87 | 102.65      | 111.57   |
| 5   | E     | 59   | THR  | N-CA-C      | -5.86 | 104.68      | 112.94   |
| 16  | P     | 303  | SER  | CA-C-N      | 5.84  | 125.94      | 119.87   |
| 16  | P     | 303  | SER  | C-N-CA      | 5.84  | 125.94      | 119.87   |
| 1   | A     | 560  | ASP  | N-CA-CB     | -5.81 | 102.13      | 110.44   |
| 1   | A     | 1203 | GLY  | CA-C-O      | -5.80 | 118.23      | 122.23   |
| 2   | B     | 246  | GLU  | CA-C-O      | -5.78 | 115.26      | 121.56   |
| 2   | B     | 301  | PRO  | N-CA-CB     | 5.76  | 109.30      | 103.25   |
| 1   | A     | 151  | ARG  | N-CA-C      | -5.74 | 105.38      | 112.38   |
| 1   | A     | 661  | ASN  | N-CA-C      | -5.71 | 106.21      | 112.72   |
| 15  | O     | 403  | PHE  | N-CA-C      | -5.71 | 105.98      | 113.12   |
| 14  | N     | 326  | VAL  | N-CA-C      | -5.68 | 107.97      | 113.53   |
| 4   | D     | 85   | GLN  | N-CA-C      | -5.66 | 105.11      | 111.28   |
| 1   | A     | 1228 | GLU  | CB-CA-C     | -5.66 | 101.73      | 110.78   |
| 19  | X     | 35   | DT   | C2'-C3'-O3' | -5.62 | 103.07      | 111.50   |
| 1   | A     | 344  | ARG  | N-CA-C      | -5.60 | 107.08      | 114.31   |
| 2   | B     | 748  | GLY  | N-CA-C      | -5.58 | 107.41      | 115.27   |
| 1   | A     | 543  | GLN  | CB-CA-C     | -5.57 | 109.66      | 117.23   |
| 14  | N     | 146  | GLU  | N-CA-C      | 5.56  | 117.14      | 111.14   |
| 17  | Q     | 78   | PRO  | N-CA-C      | -5.52 | 107.61      | 114.68   |
| 4   | D     | 59   | ARG  | N-CA-C      | -5.51 | 101.70      | 109.96   |
| 4   | D     | 19   | LEU  | N-CA-C      | -5.43 | 105.36      | 111.28   |
| 2   | B     | 507  | GLU  | N-CA-C      | 5.43  | 117.27      | 111.36   |
| 1   | A     | 128  | TYR  | N-CA-C      | -5.41 | 105.28      | 111.07   |
| 1   | A     | 534  | ASN  | N-CA-C      | -5.37 | 107.74      | 114.56   |
| 1   | A     | 371  | PRO  | N-CA-C      | 5.37  | 119.92      | 111.38   |
| 1   | A     | 419  | ASN  | CB-CA-C     | 5.36  | 118.08      | 109.07   |
| 1   | A     | 482  | PRO  | N-CA-CB     | 5.32  | 109.18      | 103.33   |
| 4   | D     | 9    | ALA  | N-CA-C      | 5.32  | 117.29      | 108.20   |
| 1   | A     | 1187 | TYR  | CB-CA-C     | 5.30  | 120.97      | 110.42   |
| 2   | B     | 354  | ARG  | N-CA-C      | -5.29 | 106.41      | 112.92   |
| 2   | B     | 507  | GLU  | CA-C-O      | -5.27 | 114.84      | 120.42   |
| 2   | B     | 397  | ALA  | N-CA-C      | -5.26 | 105.72      | 111.82   |
| 1   | A     | 39   | LYS  | N-CA-C      | 5.23  | 118.02      | 110.28   |
| 1   | A     | 622  | LYS  | N-CA-C      | -5.22 | 103.14      | 110.50   |
| 1   | A     | 1176 | THR  | CB-CA-C     | 5.20  | 115.32      | 110.17   |
| 5   | E     | 68   | PRO  | N-CA-C      | -5.19 | 106.32      | 113.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 596  | THR  | CB-CA-C     | 5.14  | 119.64      | 109.66   |
| 1   | A     | 257  | VAL  | N-CA-CB     | 5.14  | 114.86      | 110.08   |
| 3   | C     | 83   | GLU  | CA-C-N      | -5.13 | 118.89      | 122.59   |
| 3   | C     | 83   | GLU  | C-N-CA      | -5.13 | 118.89      | 122.59   |
| 11  | K     | 93   | VAL  | N-CA-C      | -5.13 | 105.54      | 110.72   |
| 5   | E     | 2    | ASP  | CA-C-N      | 5.13  | 131.33      | 121.54   |
| 5   | E     | 2    | ASP  | C-N-CA      | 5.13  | 131.33      | 121.54   |
| 2   | B     | 749  | TYR  | N-CA-C      | -5.12 | 106.88      | 113.02   |
| 20  | Y     | 2    | DC   | C5'-C4'-O4' | -5.11 | 101.73      | 109.40   |
| 2   | B     | 551  | ASP  | CB-CA-C     | -5.11 | 102.73      | 111.31   |
| 1   | A     | 1208 | SER  | CA-C-O      | -5.10 | 114.41      | 120.89   |
| 1   | A     | 576  | ASP  | N-CA-C      | -5.09 | 107.07      | 113.28   |
| 3   | C     | 170  | THR  | CB-CA-C     | 5.09  | 120.55      | 110.17   |
| 2   | B     | 587  | SER  | N-CA-C      | -5.08 | 105.40      | 112.30   |
| 1   | A     | 590  | LYS  | N-CA-CB     | 5.05  | 119.36      | 110.37   |
| 2   | B     | 94   | THR  | CB-CA-C     | 5.03  | 119.03      | 111.89   |
| 15  | O     | 376  | GLU  | CA-C-N      | 5.03  | 131.14      | 121.54   |
| 15  | O     | 376  | GLU  | C-N-CA      | 5.03  | 131.14      | 121.54   |
| 2   | B     | 742  | ALA  | CA-C-N      | -5.02 | 116.20      | 122.48   |
| 2   | B     | 742  | ALA  | C-N-CA      | -5.02 | 116.20      | 122.48   |
| 2   | B     | 553  | LYS  | CB-CA-C     | 5.01  | 119.12      | 110.79   |
| 1   | A     | 775  | ASN  | N-CA-C      | -5.01 | 101.80      | 109.76   |
| 2   | B     | 267  | PRO  | CB-CA-C     | -5.01 | 104.36      | 112.62   |

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     | 10675 | 0        | 10918    | 469     | 0            |
| 2   | B     | 8644  | 0        | 8749     | 245     | 0            |
| 3   | C     | 2736  | 0        | 2712     | 83      | 0            |
| 4   | D     | 985   | 0        | 1006     | 126     | 0            |
| 5   | E     | 1715  | 0        | 1733     | 45      | 0            |
| 6   | F     | 610   | 0        | 642      | 18      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | G     | 1337  | 0        | 1306     | 113     | 0            |
| 8   | H     | 1186  | 0        | 1147     | 31      | 0            |
| 9   | I     | 848   | 0        | 812      | 55      | 0            |
| 10  | J     | 512   | 0        | 526      | 18      | 0            |
| 11  | K     | 822   | 0        | 810      | 49      | 0            |
| 12  | L     | 388   | 0        | 395      | 16      | 0            |
| 13  | M     | 1612  | 0        | 1572     | 36      | 0            |
| 14  | N     | 1128  | 0        | 1181     | 37      | 0            |
| 15  | O     | 3546  | 0        | 3585     | 157     | 0            |
| 16  | P     | 1008  | 0        | 998      | 60      | 0            |
| 17  | Q     | 724   | 0        | 734      | 54      | 0            |
| 18  | R     | 86    | 0        | 44       | 11      | 0            |
| 19  | X     | 449   | 0        | 251      | 26      | 0            |
| 20  | Y     | 447   | 0        | 248      | 31      | 0            |
| 21  | A     | 1     | 0        | 0        | 0       | 0            |
| 22  | A     | 2     | 0        | 0        | 1       | 0            |
| 22  | B     | 1     | 0        | 0        | 1       | 0            |
| 22  | I     | 2     | 0        | 0        | 0       | 0            |
| 22  | J     | 1     | 0        | 0        | 2       | 0            |
| 22  | L     | 1     | 0        | 0        | 0       | 0            |
| 23  | P     | 8     | 0        | 0        | 4       | 0            |
| All | All   | 39474 | 0        | 39369    | 1382    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (1382) 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:1116:TYR:CE1 | 9:I:43:TYR:HE1   | 1.36                     | 1.43              |
| 8:H:76:ASN:HD21  | 11:K:87:ARG:CZ   | 1.29                     | 1.42              |
| 8:H:78:THR:CB    | 11:K:87:ARG:HH22 | 1.34                     | 1.39              |
| 1:A:1116:TYR:CE1 | 9:I:43:TYR:CE1   | 2.14                     | 1.35              |
| 1:A:1116:TYR:CD1 | 9:I:43:TYR:CE1   | 2.12                     | 1.35              |
| 1:A:1140:LEU:CD2 | 9:I:52:VAL:HG11  | 1.61                     | 1.31              |
| 1:A:1117:ILE:CG2 | 9:I:42:LYS:HB3   | 1.59                     | 1.31              |
| 1:A:1112:GLU:OE1 | 9:I:47:LYS:CD    | 1.84                     | 1.26              |
| 2:B:721:LYS:CE   | 2:B:731:GLU:OE2  | 1.84                     | 1.26              |
| 3:C:263:GLU:OE2  | 3:C:274:ARG:HD3  | 1.26                     | 1.25              |
| 2:B:721:LYS:HE2  | 2:B:731:GLU:OE2  | 1.10                     | 1.24              |
| 1:A:1119:GLU:OE1 | 9:I:40:ASN:HB3   | 1.37                     | 1.24              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:409:ILE:CD1  | 15:O:423:LEU:HD11 | 1.68                     | 1.23              |
| 15:O:356:GLU:OE1  | 17:Q:39:PRO:HD3   | 1.33                     | 1.22              |
| 15:O:374:HIS:HB3  | 15:O:423:LEU:CD1  | 1.70                     | 1.22              |
| 1:A:1118:GLU:CG   | 9:I:41:ARG:HG2    | 1.68                     | 1.21              |
| 15:O:409:ILE:CG1  | 15:O:423:LEU:HD11 | 1.68                     | 1.21              |
| 15:O:409:ILE:CG2  | 15:O:423:LEU:HD21 | 1.72                     | 1.18              |
| 15:O:410:PRO:HB2  | 15:O:419:ARG:NH2  | 1.59                     | 1.18              |
| 1:A:1140:LEU:HD23 | 9:I:52:VAL:HG11   | 1.17                     | 1.17              |
| 1:A:1118:GLU:HG2  | 9:I:41:ARG:CG     | 1.76                     | 1.16              |
| 15:O:409:ILE:HG13 | 15:O:423:LEU:CD1  | 1.76                     | 1.16              |
| 8:H:78:THR:OG1    | 11:K:87:ARG:NH2   | 1.79                     | 1.15              |
| 3:C:287:ILE:HD11  | 3:C:293:LEU:HB3   | 1.26                     | 1.15              |
| 15:O:409:ILE:H    | 15:O:410:PRO:CD   | 1.60                     | 1.13              |
| 15:O:409:ILE:HG13 | 15:O:423:LEU:HD11 | 1.28                     | 1.13              |
| 10:J:26:GLN:HA    | 10:J:26:GLN:HE21  | 1.00                     | 1.13              |
| 4:D:48:GLU:HB3    | 7:G:103:PHE:HB3   | 1.24                     | 1.12              |
| 8:H:78:THR:CB     | 11:K:87:ARG:NH2   | 2.10                     | 1.12              |
| 8:H:76:ASN:HD21   | 11:K:87:ARG:NH2   | 1.48                     | 1.11              |
| 17:Q:106:LEU:HD12 | 17:Q:107:PRO:HD2  | 1.25                     | 1.11              |
| 15:O:356:GLU:HG3  | 16:P:284:ARG:HB2  | 1.32                     | 1.11              |
| 15:O:409:ILE:N    | 15:O:410:PRO:HD2  | 1.58                     | 1.11              |
| 15:O:374:HIS:HB3  | 15:O:423:LEU:HD12 | 1.18                     | 1.11              |
| 15:O:410:PRO:CB   | 15:O:419:ARG:HH21 | 1.62                     | 1.10              |
| 1:A:1117:ILE:HG23 | 9:I:42:LYS:HB3    | 1.33                     | 1.10              |
| 8:H:76:ASN:ND2    | 11:K:87:ARG:CZ    | 2.15                     | 1.10              |
| 15:O:409:ILE:CB   | 15:O:423:LEU:HD21 | 1.83                     | 1.09              |
| 15:O:352:SER:O    | 15:O:356:GLU:HG2  | 1.51                     | 1.08              |
| 7:G:148:ILE:HG23  | 7:G:190:ILE:CG2   | 1.83                     | 1.08              |
| 10:J:10:CYS:SG    | 22:J:2000:ZN:ZN   | 1.42                     | 1.08              |
| 1:A:1112:GLU:OE1  | 9:I:47:LYS:HD3    | 0.92                     | 1.07              |
| 1:A:1117:ILE:HG23 | 9:I:42:LYS:CB     | 1.84                     | 1.07              |
| 8:H:78:THR:HB     | 11:K:87:ARG:NH1   | 1.69                     | 1.07              |
| 15:O:410:PRO:HB2  | 15:O:419:ARG:HH21 | 0.93                     | 1.07              |
| 4:D:39:GLN:HG3    | 7:G:32:LYS:HZ3    | 1.14                     | 1.06              |
| 8:H:78:THR:HB     | 11:K:87:ARG:HH12  | 1.19                     | 1.06              |
| 1:A:596:THR:HG21  | 8:H:119:GLY:O     | 1.54                     | 1.05              |
| 18:R:11:G:N2      | 20:Y:17:DC:C5     | 2.27                     | 1.03              |
| 4:D:11:LEU:HD23   | 4:D:11:LEU:H      | 1.18                     | 1.02              |
| 4:D:85:GLN:HE22   | 7:G:84:ILE:H      | 1.06                     | 1.02              |
| 16:P:299:GLY:HA2  | 16:P:303:SER:CB   | 1.89                     | 1.01              |
| 15:O:407:GLN:HB3  | 15:O:422:TYR:HB3  | 1.41                     | 1.01              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:51:LEU:HD22   | 1:A:51:LEU:H      | 1.24                     | 1.00              |
| 15:O:445:ASN:ND2  | 16:P:304:PRO:HG3  | 1.75                     | 1.00              |
| 4:D:39:GLN:HG3    | 7:G:32:LYS:CB     | 1.90                     | 1.00              |
| 15:O:409:ILE:HG21 | 15:O:423:LEU:HD21 | 1.39                     | 1.00              |
| 1:A:1117:ILE:CG2  | 9:I:42:LYS:CB     | 2.39                     | 1.00              |
| 8:H:78:THR:HB     | 11:K:87:ARG:NH2   | 1.75                     | 1.00              |
| 1:A:159:CYS:SG    | 22:A:1903:ZN:ZN   | 1.49                     | 0.99              |
| 4:D:39:GLN:CG     | 7:G:32:LYS:HB3    | 1.92                     | 0.99              |
| 1:A:1117:ILE:HG22 | 9:I:42:LYS:HB3    | 1.41                     | 0.99              |
| 4:D:39:GLN:HG3    | 7:G:32:LYS:HB3    | 0.99                     | 0.99              |
| 1:A:37:VAL:HG11   | 17:Q:28:PRO:HD3   | 1.44                     | 0.98              |
| 7:G:148:ILE:HG23  | 7:G:190:ILE:HG23  | 1.41                     | 0.98              |
| 8:H:78:THR:HB     | 11:K:87:ARG:CZ    | 1.93                     | 0.98              |
| 2:B:276:GLN:HA    | 2:B:276:GLN:HE21  | 1.25                     | 0.98              |
| 1:A:1116:TYR:HD1  | 9:I:43:TYR:CE1    | 1.73                     | 0.98              |
| 4:D:39:GLN:CG     | 7:G:32:LYS:HZ3    | 1.75                     | 0.98              |
| 1:A:180:LYS:NZ    | 1:A:182:ASN:OD1   | 1.96                     | 0.98              |
| 15:O:377:GLN:HB3  | 15:O:421:PHE:HZ   | 1.27                     | 0.97              |
| 1:A:258:PRO:HB3   | 1:A:262:ILE:HD11  | 1.47                     | 0.97              |
| 10:J:26:GLN:HA    | 10:J:26:GLN:NE2   | 1.71                     | 0.97              |
| 17:Q:27:LEU:HD22  | 17:Q:27:LEU:H     | 1.26                     | 0.96              |
| 18:R:11:G:H1      | 20:Y:17:DC:H41    | 1.13                     | 0.96              |
| 15:O:409:ILE:HD12 | 15:O:423:LEU:HD11 | 1.48                     | 0.96              |
| 16:P:300:GLY:H    | 16:P:303:SER:HB3  | 1.30                     | 0.96              |
| 20:Y:5:DC:H2''    | 20:Y:6:DT:H5'     | 1.48                     | 0.96              |
| 1:A:1140:LEU:HD23 | 9:I:52:VAL:CG1    | 1.95                     | 0.96              |
| 19:X:43:DC:C6     | 19:X:44:DT:H72    | 2.01                     | 0.95              |
| 1:A:1116:TYR:HD1  | 9:I:43:TYR:CD1    | 1.83                     | 0.95              |
| 1:A:1125:ASP:H    | 9:I:21:HIS:CE1    | 1.85                     | 0.95              |
| 15:O:409:ILE:H    | 15:O:410:PRO:HD2  | 0.79                     | 0.93              |
| 16:P:284:ARG:HA   | 16:P:284:ARG:NE   | 1.80                     | 0.93              |
| 1:A:587:THR:HG21  | 8:H:119:GLY:HA3   | 1.45                     | 0.93              |
| 12:L:34:ILE:HD12  | 12:L:34:ILE:H     | 1.34                     | 0.93              |
| 1:A:1140:LEU:CD2  | 9:I:52:VAL:CG1    | 2.47                     | 0.92              |
| 8:H:76:ASN:ND2    | 11:K:87:ARG:NH2   | 2.14                     | 0.92              |
| 16:P:299:GLY:HA2  | 16:P:303:SER:HB3  | 1.51                     | 0.92              |
| 15:O:412:THR:HB   | 15:O:419:ARG:HA   | 1.50                     | 0.92              |
| 3:C:288:PHE:HA    | 3:C:294:LYS:HG2   | 1.53                     | 0.91              |
| 4:D:85:GLN:NE2    | 7:G:83:GLU:HA     | 1.84                     | 0.91              |
| 2:B:306:ILE:HD13  | 2:B:306:ILE:H     | 1.36                     | 0.91              |
| 8:H:78:THR:HB     | 11:K:87:ARG:HH22  | 1.28                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:249:GLN:HE22  | 14:N:144:LYS:HE3  | 1.35                     | 0.91              |
| 15:O:409:ILE:HB   | 15:O:423:LEU:HD21 | 1.49                     | 0.91              |
| 18:R:11:G:H22     | 20:Y:17:DC:H5     | 1.19                     | 0.91              |
| 4:D:17:PHE:HB2    | 4:D:53:ILE:HG21   | 1.53                     | 0.91              |
| 1:A:1116:TYR:CD1  | 9:I:43:TYR:CD1    | 2.58                     | 0.90              |
| 2:B:282:GLN:NE2   | 13:M:146:ASP:OD2  | 2.04                     | 0.90              |
| 4:D:11:LEU:H      | 4:D:11:LEU:CD2    | 1.84                     | 0.90              |
| 4:D:4:LYS:HE2     | 4:D:4:LYS:HA      | 1.52                     | 0.90              |
| 5:E:61:LEU:H      | 5:E:61:LEU:HD22   | 1.35                     | 0.90              |
| 16:P:284:ARG:HA   | 16:P:284:ARG:HE   | 1.33                     | 0.90              |
| 3:C:9:GLU:OE2     | 3:C:298:ARG:NH1   | 2.05                     | 0.90              |
| 4:D:97:ILE:HA     | 4:D:101:VAL:HB    | 1.54                     | 0.89              |
| 17:Q:106:LEU:HD12 | 17:Q:107:PRO:CD   | 2.00                     | 0.89              |
| 15:O:407:GLN:O    | 15:O:410:PRO:HD2  | 1.73                     | 0.89              |
| 1:A:1116:TYR:HE1  | 9:I:43:TYR:HE1    | 0.88                     | 0.88              |
| 4:D:48:GLU:CB     | 7:G:103:PHE:HB3   | 2.04                     | 0.87              |
| 17:Q:27:LEU:H     | 17:Q:27:LEU:CD2   | 1.86                     | 0.87              |
| 4:D:48:GLU:HB3    | 7:G:103:PHE:O     | 1.74                     | 0.86              |
| 10:J:10:CYS:HG    | 22:J:2000:ZN:ZN   | 0.55                     | 0.86              |
| 1:A:1143:GLU:OE2  | 5:E:2:ASP:OD1     | 1.91                     | 0.86              |
| 1:A:1112:GLU:CD   | 9:I:47:LYS:HD3    | 2.00                     | 0.85              |
| 1:A:461:LEU:HD21  | 2:B:1063:LEU:HD21 | 1.58                     | 0.85              |
| 4:D:11:LEU:HD21   | 7:G:3:VAL:HA      | 1.58                     | 0.85              |
| 15:O:377:GLN:HB3  | 15:O:421:PHE:CZ   | 2.10                     | 0.85              |
| 15:O:407:GLN:O    | 15:O:410:PRO:CD   | 2.24                     | 0.85              |
| 4:D:43:ASN:H      | 4:D:43:ASN:HD22   | 1.25                     | 0.85              |
| 15:O:374:HIS:CB   | 15:O:423:LEU:HD12 | 2.06                     | 0.85              |
| 1:A:1146:ALA:HB2  | 1:A:1171:ALA:HA   | 1.58                     | 0.84              |
| 15:O:409:ILE:HG13 | 15:O:423:LEU:CG   | 2.06                     | 0.84              |
| 2:B:276:GLN:HA    | 2:B:276:GLN:NE2   | 1.90                     | 0.83              |
| 4:D:58:CYS:HA     | 4:D:61:GLN:HB2    | 1.60                     | 0.83              |
| 18:R:11:G:N2      | 20:Y:17:DC:H5     | 1.72                     | 0.83              |
| 1:A:1092:ASP:OD1  | 1:A:1092:ASP:N    | 2.11                     | 0.83              |
| 4:D:11:LEU:HD23   | 4:D:11:LEU:N      | 1.91                     | 0.83              |
| 2:B:25:GLU:OE2    | 2:B:25:GLU:HA     | 1.79                     | 0.82              |
| 3:C:287:ILE:CD1   | 3:C:293:LEU:HB3   | 2.09                     | 0.82              |
| 8:H:78:THR:CB     | 11:K:87:ARG:HH12  | 1.91                     | 0.82              |
| 15:O:415:HIS:O    | 15:O:419:ARG:HG3  | 1.78                     | 0.82              |
| 5:E:111:THR:HG21  | 19:X:44:DT:OP2    | 1.79                     | 0.82              |
| 1:A:1116:TYR:HE1  | 9:I:43:TYR:CE1    | 1.77                     | 0.82              |
| 1:A:196:SER:HB2   | 15:O:373:LYS:HE3  | 1.62                     | 0.82              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:991:SER:HB2   | 2:B:998:LEU:HD21 | 1.61                     | 0.81              |
| 7:G:148:ILE:HG23  | 7:G:190:ILE:HG21 | 1.60                     | 0.81              |
| 15:O:409:ILE:HB   | 15:O:423:LEU:CD2 | 2.09                     | 0.81              |
| 1:A:115:ILE:HD11  | 1:A:234:ASP:O    | 1.80                     | 0.81              |
| 1:A:1051:LYS:HE3  | 1:A:1051:LYS:O   | 1.80                     | 0.81              |
| 16:P:299:GLY:HA2  | 16:P:303:SER:HB2 | 1.61                     | 0.81              |
| 19:X:37:DG:H2'    | 19:X:38:DA:C8    | 2.16                     | 0.81              |
| 2:B:507:GLU:CD    | 2:B:507:GLU:H    | 1.87                     | 0.81              |
| 15:O:407:GLN:CB   | 15:O:422:TYR:HB3 | 2.10                     | 0.81              |
| 4:D:39:GLN:CG     | 7:G:32:LYS:NZ    | 2.43                     | 0.80              |
| 4:D:85:GLN:HE22   | 7:G:84:ILE:N     | 1.77                     | 0.80              |
| 3:C:263:GLU:OE2   | 3:C:274:ARG:CD   | 2.21                     | 0.80              |
| 3:C:287:ILE:HD11  | 3:C:293:LEU:CB   | 2.10                     | 0.80              |
| 1:A:1261:GLU:HG3  | 5:E:193:ILE:HD13 | 1.61                     | 0.80              |
| 3:C:78:ARG:HE     | 11:K:50:THR:HG22 | 1.46                     | 0.80              |
| 19:X:39:DG:H2''   | 19:X:40:DC:H5'   | 1.62                     | 0.79              |
| 4:D:39:GLN:HG3    | 7:G:32:LYS:NZ    | 1.97                     | 0.79              |
| 1:A:1121:PHE:HE2  | 9:I:14:VAL:HG21  | 1.46                     | 0.79              |
| 1:A:1117:ILE:HG23 | 9:I:42:LYS:HB2   | 1.64                     | 0.78              |
| 1:A:1118:GLU:HG2  | 9:I:41:ARG:HG2   | 0.85                     | 0.78              |
| 4:D:48:GLU:OE1    | 7:G:103:PHE:CG   | 2.35                     | 0.78              |
| 1:A:587:THR:CG2   | 8:H:119:GLY:HA3  | 2.13                     | 0.78              |
| 15:O:356:GLU:CG   | 16:P:284:ARG:HB2 | 2.13                     | 0.78              |
| 1:A:59:ARG:HG3    | 1:A:70:GLU:HB2   | 1.65                     | 0.77              |
| 2:B:213:ARG:HB3   | 2:B:213:ARG:HH21 | 1.49                     | 0.77              |
| 4:D:10:LEU:HD23   | 4:D:10:LEU:O     | 1.83                     | 0.77              |
| 1:A:1112:GLU:O    | 9:I:46:LEU:CD2   | 2.32                     | 0.77              |
| 16:P:300:GLY:N    | 16:P:303:SER:HB3 | 1.97                     | 0.77              |
| 2:B:361:ARG:HD2   | 2:B:591:ARG:HG2  | 1.64                     | 0.77              |
| 4:D:54:SER:HA     | 4:D:59:ARG:NH1   | 2.00                     | 0.77              |
| 1:A:1055:PHE:HA   | 1:A:1062:ASN:HA  | 1.67                     | 0.76              |
| 2:B:578:LEU:HD23  | 2:B:578:LEU:H    | 1.49                     | 0.76              |
| 1:A:322:ASN:C     | 1:A:322:ASN:HD22 | 1.93                     | 0.76              |
| 4:D:107:ARG:HH21  | 17:Q:82:GLN:CD   | 1.92                     | 0.76              |
| 15:O:445:ASN:OD1  | 23:P:401:SF4:S2  | 2.43                     | 0.76              |
| 5:E:79:GLU:H      | 5:E:79:GLU:CD    | 1.92                     | 0.76              |
| 7:G:151:ARG:HD2   | 7:G:151:ARG:O    | 1.85                     | 0.76              |
| 3:C:239:ILE:HD12  | 3:C:239:ILE:H    | 1.50                     | 0.76              |
| 1:A:1233:ARG:HD3  | 5:E:134:GLU:HG2  | 1.67                     | 0.76              |
| 2:B:721:LYS:NZ    | 2:B:731:GLU:OE2  | 2.19                     | 0.75              |
| 4:D:45:ILE:HB     | 7:G:36:ASN:OD1   | 1.85                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 17:Q:106:LEU:CD1 | 17:Q:107:PRO:HD2 | 2.13                     | 0.75              |
| 2:B:236:ILE:HA   | 2:B:239:ILE:HD12 | 1.68                     | 0.75              |
| 17:Q:27:LEU:HD22 | 17:Q:27:LEU:N    | 2.00                     | 0.75              |
| 19:X:24:DT:H2'   | 19:X:24:DT:O2    | 1.87                     | 0.75              |
| 5:E:84:ILE:HD12  | 5:E:84:ILE:H     | 1.51                     | 0.75              |
| 1:A:586:PRO:HG3  | 1:A:595:TRP:CZ2  | 2.21                     | 0.75              |
| 1:A:1119:GLU:CD  | 1:A:1119:GLU:H   | 1.94                     | 0.75              |
| 2:B:506:MET:HG3  | 2:B:587:SER:HB2  | 1.68                     | 0.75              |
| 6:F:82:GLU:O     | 6:F:82:GLU:HG2   | 1.84                     | 0.75              |
| 1:A:1112:GLU:O   | 9:I:46:LEU:HD23  | 1.87                     | 0.75              |
| 3:C:65:MET:HE2   | 3:C:68:ILE:HG21  | 1.69                     | 0.74              |
| 15:O:356:GLU:OE1 | 17:Q:39:PRO:CD   | 2.26                     | 0.74              |
| 16:P:293:PHE:HE2 | 16:P:307:CYS:HB2 | 1.51                     | 0.74              |
| 2:B:995:GLY:O    | 3:C:233:TYR:OH   | 2.04                     | 0.74              |
| 3:C:288:PHE:O    | 3:C:294:LYS:HD3  | 1.87                     | 0.74              |
| 7:G:99:VAL:HG21  | 7:G:148:ILE:HD11 | 1.70                     | 0.74              |
| 2:B:619:ARG:CZ   | 2:B:619:ARG:HB3  | 2.17                     | 0.74              |
| 12:L:25:GLU:H    | 12:L:25:GLU:CD   | 1.95                     | 0.74              |
| 3:C:163:TYR:CE1  | 3:C:204:PRO:HD3  | 2.23                     | 0.74              |
| 4:D:48:GLU:CB    | 7:G:103:PHE:O    | 2.35                     | 0.74              |
| 7:G:32:LYS:HZ3   | 7:G:32:LYS:HB3   | 1.52                     | 0.74              |
| 8:H:78:THR:HG1   | 11:K:87:ARG:NH2  | 1.83                     | 0.74              |
| 1:A:45:ASP:HB2   | 1:A:50:PRO:HD2   | 1.68                     | 0.73              |
| 7:G:79:PRO:HG2   | 7:G:150:PHE:CE2  | 2.24                     | 0.73              |
| 1:A:98:PHE:HE2   | 1:A:168:LYS:HD3  | 1.53                     | 0.73              |
| 1:A:1121:PHE:CE2 | 9:I:14:VAL:HG21  | 2.23                     | 0.73              |
| 5:E:55:ARG:H     | 5:E:55:ARG:HD3   | 1.52                     | 0.73              |
| 2:B:542:ASN:N    | 2:B:542:ASN:HD22 | 1.86                     | 0.73              |
| 3:C:163:TYR:CD1  | 3:C:204:PRO:HD3  | 2.24                     | 0.73              |
| 1:A:17:HIS:CD2   | 1:A:1337:LYS:HG3 | 2.24                     | 0.72              |
| 1:A:544:ASP:HA   | 1:A:547:THR:HG22 | 1.70                     | 0.72              |
| 4:D:77:LYS:O     | 4:D:77:LYS:HG3   | 1.90                     | 0.72              |
| 3:C:135:ILE:H    | 3:C:135:ILE:HD12 | 1.54                     | 0.72              |
| 12:L:26:ASN:HB2  | 12:L:44:MET:HE1  | 1.71                     | 0.72              |
| 8:H:78:THR:CB    | 11:K:87:ARG:NH1  | 2.50                     | 0.71              |
| 15:O:357:ARG:NH1 | 16:P:288:GLY:O   | 2.23                     | 0.71              |
| 2:B:236:ILE:HD11 | 2:B:265:PHE:HE1  | 1.55                     | 0.71              |
| 2:B:249:GLN:HE22 | 14:N:144:LYS:CE  | 2.02                     | 0.71              |
| 1:A:941:SER:HB3  | 1:A:980:ILE:HG21 | 1.72                     | 0.71              |
| 2:B:874:ASN:OD1  | 2:B:874:ASN:N    | 2.23                     | 0.71              |
| 7:G:151:ARG:HD2  | 7:G:151:ARG:C    | 2.16                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:1:MET:HA      | 4:D:1:MET:HE2     | 1.71                     | 0.70              |
| 1:A:115:ILE:HG13  | 1:A:234:ASP:HB3   | 1.71                     | 0.70              |
| 1:A:303:THR:H     | 15:O:377:GLN:HE22 | 1.38                     | 0.70              |
| 13:M:227:CYS:O    | 13:M:228:PRO:C    | 2.34                     | 0.70              |
| 4:D:39:GLN:HG2    | 7:G:32:LYS:NZ     | 2.07                     | 0.69              |
| 1:A:738:GLN:HA    | 1:A:747:THR:HG21  | 1.74                     | 0.69              |
| 5:E:111:THR:CG2   | 19:X:44:DT:OP2    | 2.41                     | 0.69              |
| 1:A:36:VAL:O      | 1:A:36:VAL:HG12   | 1.93                     | 0.69              |
| 2:B:733:LEU:HD23  | 2:B:733:LEU:H     | 1.58                     | 0.69              |
| 4:D:1:MET:O       | 4:D:1:MET:SD      | 2.51                     | 0.69              |
| 20:Y:10:DG:H2''   | 20:Y:11:DT:H5'    | 1.73                     | 0.69              |
| 15:O:356:GLU:HG3  | 16:P:284:ARG:CB   | 2.18                     | 0.69              |
| 15:O:409:ILE:HG21 | 15:O:423:LEU:CD2  | 2.18                     | 0.69              |
| 20:Y:11:DT:H2''   | 20:Y:12:DC:C5     | 2.28                     | 0.69              |
| 1:A:51:LEU:HD13   | 1:A:51:LEU:N      | 2.08                     | 0.68              |
| 1:A:1129:LEU:O    | 1:A:1129:LEU:HD23 | 1.93                     | 0.68              |
| 8:H:76:ASN:HD21   | 11:K:87:ARG:NE    | 1.88                     | 0.68              |
| 15:O:409:ILE:HG13 | 15:O:423:LEU:HG   | 1.75                     | 0.68              |
| 1:A:119:GLN:OE1   | 1:A:119:GLN:N     | 2.26                     | 0.68              |
| 4:D:48:GLU:HB3    | 7:G:103:PHE:CB    | 2.15                     | 0.68              |
| 1:A:479:ARG:NH2   | 1:A:479:ARG:HB3   | 2.09                     | 0.68              |
| 1:A:822:GLU:CD    | 1:A:822:GLU:H     | 2.01                     | 0.68              |
| 2:B:236:ILE:HD11  | 2:B:265:PHE:CE1   | 2.28                     | 0.68              |
| 1:A:816:ARG:HD3   | 1:A:823:LYS:HG2   | 1.75                     | 0.68              |
| 1:A:1230:ASP:OD1  | 1:A:1230:ASP:N    | 2.25                     | 0.68              |
| 5:E:47:LYS:N      | 5:E:48:PRO:HD2    | 2.09                     | 0.68              |
| 5:E:55:ARG:HD3    | 5:E:55:ARG:N      | 2.09                     | 0.68              |
| 1:A:102:ILE:HD13  | 1:A:168:LYS:HB2   | 1.75                     | 0.67              |
| 2:B:119:TYR:HD1   | 2:B:119:TYR:H     | 1.40                     | 0.67              |
| 1:A:213:ARG:H     | 1:A:213:ARG:HD2   | 1.59                     | 0.67              |
| 16:P:299:GLY:CA   | 16:P:303:SER:HB3  | 2.24                     | 0.67              |
| 2:B:30:LEU:HD13   | 2:B:499:MET:HG3   | 1.74                     | 0.67              |
| 15:O:357:ARG:HG2  | 16:P:289:LEU:HA   | 1.76                     | 0.67              |
| 15:O:412:THR:CB   | 15:O:419:ARG:HA   | 2.24                     | 0.67              |
| 1:A:880:GLU:HG3   | 1:A:1343:VAL:HG22 | 1.75                     | 0.67              |
| 15:O:445:ASN:HD22 | 16:P:304:PRO:HG3  | 1.59                     | 0.67              |
| 19:X:43:DC:N3     | 20:Y:1:DG:N2      | 2.40                     | 0.67              |
| 1:A:5:GLN:OE1     | 1:A:5:GLN:N       | 2.27                     | 0.66              |
| 20:Y:11:DT:H2'    | 20:Y:11:DT:O2     | 1.95                     | 0.66              |
| 1:A:1128:ILE:HG23 | 1:A:1176:THR:HG23 | 1.76                     | 0.66              |
| 13:M:238:LEU:HD13 | 14:N:341:LEU:HG   | 1.77                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:26:GLN:HE21  | 10:J:26:GLN:CA    | 1.82                     | 0.66              |
| 20:Y:12:DC:H2'    | 20:Y:13:DT:H71    | 1.78                     | 0.66              |
| 13:M:49:ILE:HD13  | 14:N:363:VAL:HG11 | 1.78                     | 0.65              |
| 1:A:213:ARG:HD2   | 1:A:213:ARG:N     | 2.12                     | 0.65              |
| 2:B:59:MET:HE2    | 2:B:80:ILE:HG13   | 1.78                     | 0.65              |
| 1:A:154:ASN:HB3   | 1:A:162:PHE:HE1   | 1.61                     | 0.65              |
| 1:A:942:LYS:HD3   | 1:A:981:LYS:HB2   | 1.79                     | 0.65              |
| 1:A:224:LEU:HD22  | 1:A:228:LYS:HE3   | 1.78                     | 0.65              |
| 2:B:259:GLU:H     | 2:B:259:GLU:CD    | 2.04                     | 0.65              |
| 2:B:733:LEU:HD23  | 2:B:733:LEU:N     | 2.11                     | 0.65              |
| 1:A:383:PRO:HB3   | 1:A:484:ARG:HA    | 1.79                     | 0.65              |
| 1:A:479:ARG:HB3   | 1:A:479:ARG:HH21  | 1.60                     | 0.65              |
| 2:B:364:LEU:HD21  | 2:B:502:ILE:HD12  | 1.78                     | 0.65              |
| 2:B:242:ALA:HB1   | 2:B:284:LEU:HD23  | 1.78                     | 0.65              |
| 17:Q:86:ARG:NH1   | 17:Q:86:ARG:HB2   | 2.12                     | 0.65              |
| 5:E:84:ILE:HD13   | 19:X:44:DT:H3'    | 1.77                     | 0.65              |
| 10:J:26:GLN:NE2   | 10:J:26:GLN:CA    | 2.49                     | 0.65              |
| 1:A:1178:ARG:HG3  | 1:A:1189:LEU:HD21 | 1.78                     | 0.64              |
| 1:A:438:GLU:OE1   | 1:A:438:GLU:N     | 2.27                     | 0.64              |
| 2:B:23:VAL:O      | 2:B:23:VAL:HG23   | 1.97                     | 0.64              |
| 3:C:139:GLN:HG2   | 3:C:211:LEU:HD11  | 1.79                     | 0.64              |
| 1:A:193:PHE:CD1   | 1:A:193:PHE:C     | 2.76                     | 0.64              |
| 1:A:997:PRO:HB2   | 1:A:1000:LEU:HD23 | 1.78                     | 0.63              |
| 1:A:1094:ASP:OD1  | 1:A:1094:ASP:N    | 2.32                     | 0.63              |
| 4:D:73:LEU:HD13   | 4:D:83:LYS:HB2    | 1.78                     | 0.63              |
| 16:P:220:ILE:HD11 | 16:P:271:ARG:HD2  | 1.80                     | 0.63              |
| 1:A:38:SER:HB2    | 1:A:54:GLY:HA2    | 1.78                     | 0.63              |
| 1:A:386:VAL:HG23  | 2:B:1020:MET:HE2  | 1.80                     | 0.63              |
| 3:C:288:PHE:HA    | 3:C:294:LYS:CG    | 2.27                     | 0.63              |
| 4:D:41:ASN:OD1    | 4:D:41:ASN:N      | 2.30                     | 0.63              |
| 16:P:293:PHE:CE1  | 17:Q:31:VAL:HG12  | 2.33                     | 0.63              |
| 1:A:17:HIS:CD2    | 1:A:17:HIS:O      | 2.52                     | 0.63              |
| 2:B:750:ASP:HA    | 2:B:754:ALA:HB3   | 1.80                     | 0.63              |
| 4:D:107:ARG:NH2   | 17:Q:82:GLN:HG2   | 2.13                     | 0.63              |
| 12:L:34:ILE:HG22  | 12:L:44:MET:HG3   | 1.80                     | 0.63              |
| 1:A:17:HIS:HB2    | 1:A:1337:LYS:HE2  | 1.80                     | 0.63              |
| 1:A:1048:MET:HA   | 1:A:1280:MET:CE   | 2.28                     | 0.63              |
| 4:D:17:PHE:HB2    | 4:D:53:ILE:CG2    | 2.28                     | 0.63              |
| 15:O:407:GLN:CG   | 15:O:422:TYR:HB3  | 2.29                     | 0.63              |
| 1:A:569:ALA:HA    | 1:A:572:LEU:HD12  | 1.80                     | 0.63              |
| 3:C:270:LYS:NZ    | 3:C:270:LYS:HB3   | 2.13                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:864:LYS:HZ2  | 1:A:1048:MET:HB2 | 1.63                     | 0.63              |
| 11:K:58:MET:HE3  | 11:K:58:MET:HA   | 1.81                     | 0.63              |
| 2:B:1083:CYS:SG  | 22:B:1201:ZN:ZN  | 1.88                     | 0.63              |
| 1:A:193:PHE:C    | 1:A:193:PHE:HD1  | 2.07                     | 0.62              |
| 2:B:204:THR:HG23 | 2:B:213:ARG:HG2  | 1.81                     | 0.62              |
| 2:B:527:CYS:O    | 2:B:527:CYS:SG   | 2.57                     | 0.62              |
| 3:C:54:VAL:CG1   | 3:C:62:GLU:HG2   | 2.29                     | 0.62              |
| 1:A:53:TYR:O     | 1:A:53:TYR:HD1   | 1.81                     | 0.62              |
| 1:A:136:TYR:HD1  | 1:A:136:TYR:O    | 1.81                     | 0.62              |
| 1:A:171:LEU:HD22 | 1:A:327:GLY:O    | 1.99                     | 0.62              |
| 3:C:102:GLN:OE1  | 3:C:102:GLN:N    | 2.32                     | 0.62              |
| 4:D:2:GLU:H      | 4:D:2:GLU:CD     | 2.07                     | 0.62              |
| 7:G:79:PRO:CG    | 7:G:150:PHE:CE2  | 2.82                     | 0.62              |
| 4:D:107:ARG:HH21 | 17:Q:82:GLN:CG   | 2.12                     | 0.62              |
| 13:M:248:MET:HE1 | 14:N:276:PRO:HA  | 1.81                     | 0.62              |
| 15:O:159:ARG:HA  | 15:O:235:TRP:HB3 | 1.80                     | 0.62              |
| 1:A:328:ILE:HD12 | 1:A:328:ILE:H    | 1.64                     | 0.62              |
| 1:A:484:ARG:HH11 | 1:A:484:ARG:HB3  | 1.64                     | 0.62              |
| 2:B:507:GLU:CD   | 2:B:507:GLU:N    | 2.58                     | 0.62              |
| 2:B:1095:CYS:O   | 2:B:1097:SER:N   | 2.28                     | 0.62              |
| 1:A:98:PHE:CE2   | 1:A:168:LYS:HD3  | 2.34                     | 0.62              |
| 2:B:549:ILE:HD12 | 2:B:549:ILE:O    | 2.00                     | 0.62              |
| 2:B:991:SER:HB2  | 2:B:998:LEU:CD2  | 2.29                     | 0.62              |
| 3:C:134:GLU:HG2  | 3:C:181:GLN:HG3  | 1.82                     | 0.62              |
| 1:A:197:PHE:HD1  | 1:A:197:PHE:O    | 1.82                     | 0.62              |
| 1:A:1112:GLU:O   | 9:I:46:LEU:HD22  | 2.00                     | 0.62              |
| 4:D:14:TYR:HD2   | 4:D:18:GLN:HE21  | 1.47                     | 0.62              |
| 18:R:10:U:H3'    | 18:R:11:G:H8     | 1.65                     | 0.62              |
| 1:A:1369:ASP:OD1 | 7:G:23:ASN:ND2   | 2.33                     | 0.61              |
| 2:B:685:TYR:HB3  | 2:B:689:MET:HE3  | 1.81                     | 0.61              |
| 1:A:322:ASN:C    | 1:A:322:ASN:ND2  | 2.58                     | 0.61              |
| 16:P:199:LYS:NZ  | 16:P:245:ASP:O   | 2.32                     | 0.61              |
| 1:A:107:MET:O    | 1:A:116:MET:HG2  | 1.99                     | 0.61              |
| 1:A:474:MET:HE1  | 1:A:539:ILE:HD11 | 1.81                     | 0.61              |
| 3:C:187:GLU:H    | 3:C:187:GLU:CD   | 2.09                     | 0.61              |
| 4:D:20:LEU:HD11  | 4:D:46:THR:HB    | 1.82                     | 0.61              |
| 8:H:78:THR:CB    | 11:K:87:ARG:CZ   | 2.66                     | 0.61              |
| 16:P:293:PHE:CE2 | 16:P:307:CYS:HB2 | 2.34                     | 0.61              |
| 1:A:1360:PHE:CZ  | 6:F:61:GLU:HA    | 2.35                     | 0.61              |
| 1:A:1118:GLU:HA  | 9:I:40:ASN:O     | 2.01                     | 0.61              |
| 7:G:151:ARG:HG3  | 7:G:152:VAL:HG13 | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:57:ASP:C      | 1:A:59:ARG:H      | 2.08                     | 0.61              |
| 1:A:591:PRO:HG2   | 8:H:47:ILE:HD12   | 1.82                     | 0.61              |
| 1:A:822:GLU:HG2   | 1:A:825:SER:HB2   | 1.82                     | 0.61              |
| 15:O:91:TYR:OH    | 15:O:243:HIS:NE2  | 2.33                     | 0.61              |
| 1:A:51:LEU:H      | 1:A:51:LEU:CD2    | 1.95                     | 0.60              |
| 2:B:876:GLU:OE1   | 2:B:876:GLU:N     | 2.31                     | 0.60              |
| 15:O:507:ASN:ND2  | 17:Q:55:GLU:OE2   | 2.34                     | 0.60              |
| 1:A:7:ARG:HD3     | 1:A:7:ARG:C       | 2.27                     | 0.60              |
| 1:A:149:LYS:O     | 1:A:153:LYS:HG3   | 2.01                     | 0.60              |
| 2:B:758:ASN:HB3   | 2:B:916:MET:SD    | 2.40                     | 0.60              |
| 16:P:302:ILE:HG22 | 16:P:302:ILE:O    | 2.00                     | 0.60              |
| 1:A:48:HIS:CG     | 1:A:48:HIS:O      | 2.54                     | 0.60              |
| 1:A:1120:VAL:HG22 | 9:I:39:THR:HG22   | 1.84                     | 0.60              |
| 1:A:57:ASP:O      | 1:A:59:ARG:N      | 2.35                     | 0.60              |
| 1:A:102:ILE:HG23  | 1:A:166:VAL:HG12  | 1.84                     | 0.60              |
| 2:B:916:MET:HG2   | 2:B:925:PRO:HD2   | 1.84                     | 0.60              |
| 2:B:348:ASP:OD1   | 2:B:348:ASP:N     | 2.32                     | 0.60              |
| 1:A:120:GLU:CD    | 1:A:120:GLU:C     | 2.70                     | 0.60              |
| 1:A:985:ASP:HA    | 1:A:989:ILE:HG12  | 1.83                     | 0.60              |
| 1:A:1261:GLU:OE2  | 5:E:207:ARG:NH2   | 2.31                     | 0.60              |
| 12:L:34:ILE:HD12  | 12:L:34:ILE:N     | 2.12                     | 0.60              |
| 1:A:38:SER:C      | 17:Q:24:GLY:HA2   | 2.27                     | 0.60              |
| 1:A:1073:ILE:HG21 | 1:A:1271:ILE:HG13 | 1.84                     | 0.60              |
| 1:A:414:VAL:HG12  | 1:A:416:PRO:HD2   | 1.84                     | 0.60              |
| 2:B:542:ASN:HD22  | 2:B:542:ASN:H     | 1.48                     | 0.60              |
| 1:A:7:ARG:N       | 7:G:38:VAL:O      | 2.29                     | 0.59              |
| 1:A:953:MET:HA    | 1:A:953:MET:HE2   | 1.85                     | 0.59              |
| 1:A:1087:ALA:HB3  | 1:A:1225:LEU:HD12 | 1.84                     | 0.59              |
| 1:A:1159:ARG:NH1  | 19:X:41:DC:OP1    | 2.35                     | 0.59              |
| 1:A:1208:SER:O    | 1:A:1209:ARG:HB2  | 2.01                     | 0.59              |
| 4:D:107:ARG:HH21  | 17:Q:82:GLN:HG2   | 1.66                     | 0.59              |
| 1:A:1048:MET:CB   | 1:A:1280:MET:HE1  | 2.32                     | 0.59              |
| 1:A:1128:ILE:HD13 | 1:A:1128:ILE:C    | 2.27                     | 0.59              |
| 4:D:108:LEU:O     | 4:D:113:ILE:HG22  | 2.02                     | 0.59              |
| 10:J:19:GLU:CD    | 10:J:19:GLU:H     | 2.09                     | 0.59              |
| 1:A:136:TYR:CD1   | 1:A:136:TYR:C     | 2.81                     | 0.59              |
| 1:A:1220:LYS:O    | 1:A:1220:LYS:HG2  | 2.02                     | 0.59              |
| 2:B:59:MET:HE1    | 2:B:78:LEU:C      | 2.26                     | 0.59              |
| 4:D:1:MET:O       | 4:D:1:MET:CG      | 2.51                     | 0.59              |
| 4:D:9:ALA:HB2     | 7:G:3:VAL:HG23    | 1.85                     | 0.59              |
| 17:Q:80:GLU:HA    | 17:Q:86:ARG:CD    | 2.33                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1122:LEU:HG   | 1:A:1123:PRO:HD2  | 1.84                     | 0.59              |
| 3:C:54:VAL:HG11   | 3:C:62:GLU:HG2    | 1.85                     | 0.59              |
| 7:G:79:PRO:CG     | 7:G:150:PHE:CD2   | 2.86                     | 0.59              |
| 1:A:84:GLY:O      | 1:A:257:VAL:N     | 2.33                     | 0.59              |
| 15:O:445:ASN:HD21 | 16:P:304:PRO:HG3  | 1.64                     | 0.59              |
| 1:A:586:PRO:HG3   | 1:A:595:TRP:CH2   | 2.37                     | 0.59              |
| 1:A:1155:THR:HG23 | 1:A:1155:THR:O    | 2.02                     | 0.59              |
| 2:B:1095:CYS:O    | 2:B:1095:CYS:SG   | 2.61                     | 0.59              |
| 15:O:364:ARG:NH2  | 15:O:384:ALA:O    | 2.35                     | 0.59              |
| 1:A:737:GLN:N     | 1:A:737:GLN:OE1   | 2.34                     | 0.59              |
| 1:A:1140:LEU:HD21 | 9:I:52:VAL:HG11   | 1.75                     | 0.59              |
| 1:A:53:TYR:O      | 1:A:53:TYR:CD1    | 2.56                     | 0.58              |
| 3:C:163:TYR:CE1   | 3:C:204:PRO:CD    | 2.86                     | 0.58              |
| 4:D:7:ASN:HD22    | 17:Q:78:PRO:HG3   | 1.67                     | 0.58              |
| 4:D:110:GLU:OE2   | 4:D:110:GLU:HA    | 2.01                     | 0.58              |
| 15:O:356:GLU:OE2  | 16:P:282:LEU:HD22 | 2.03                     | 0.58              |
| 3:C:183:ASP:OD1   | 3:C:183:ASP:N     | 2.35                     | 0.58              |
| 4:D:18:GLN:OE1    | 4:D:18:GLN:HA     | 2.02                     | 0.58              |
| 2:B:24:GLU:OE1    | 2:B:24:GLU:HA     | 2.04                     | 0.58              |
| 3:C:139:GLN:HB2   | 3:C:178:LEU:HD11  | 1.85                     | 0.58              |
| 1:A:102:ILE:HG12  | 1:A:174:ILE:HG12  | 1.86                     | 0.58              |
| 1:A:166:VAL:HG13  | 1:A:174:ILE:HG23  | 1.85                     | 0.58              |
| 2:B:88:GLU:H      | 2:B:88:GLU:CD     | 2.11                     | 0.58              |
| 2:B:259:GLU:OE1   | 2:B:259:GLU:N     | 2.27                     | 0.58              |
| 1:A:17:HIS:CD2    | 1:A:1337:LYS:CG   | 2.87                     | 0.58              |
| 3:C:316:LEU:N     | 3:C:316:LEU:HD23  | 2.18                     | 0.58              |
| 1:A:136:TYR:HD1   | 1:A:136:TYR:C     | 2.12                     | 0.58              |
| 15:O:284:PHE:HA   | 15:O:338:LEU:HB2  | 1.84                     | 0.58              |
| 2:B:1051:GLU:OE1  | 2:B:1051:GLU:N    | 2.31                     | 0.58              |
| 7:G:114:LEU:HD21  | 7:G:192:GLU:H     | 1.68                     | 0.58              |
| 1:A:58:HIS:O      | 1:A:70:GLU:HG2    | 2.04                     | 0.58              |
| 1:A:1076:ALA:HB3  | 1:A:1302:GLY:HA3  | 1.86                     | 0.58              |
| 17:Q:113:ARG:HH21 | 17:Q:117:LYS:HA   | 1.67                     | 0.58              |
| 1:A:331:ASN:O     | 1:A:331:ASN:ND2   | 2.37                     | 0.58              |
| 4:D:43:ASN:H      | 4:D:43:ASN:ND2    | 1.96                     | 0.58              |
| 4:D:54:SER:HA     | 4:D:59:ARG:CZ     | 2.34                     | 0.58              |
| 7:G:112:GLU:OE1   | 7:G:119:LYS:NZ    | 2.37                     | 0.58              |
| 8:H:78:THR:CG2    | 11:K:87:ARG:HH12  | 2.17                     | 0.58              |
| 1:A:587:THR:HG23  | 1:A:599:GLN:CD    | 2.28                     | 0.57              |
| 2:B:396:ARG:NH1   | 2:B:396:ARG:HB2   | 2.19                     | 0.57              |
| 15:O:410:PRO:CB   | 15:O:419:ARG:NH2  | 2.40                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:Y:17:DC:H2'    | 20:Y:18:DA:O4'    | 2.03                     | 0.57              |
| 1:A:137:LEU:HD21  | 1:A:1310:LYS:HA   | 1.85                     | 0.57              |
| 1:A:1242:LYS:O    | 1:A:1242:LYS:HG3  | 2.01                     | 0.57              |
| 2:B:721:LYS:NZ    | 2:B:731:GLU:CD    | 2.62                     | 0.57              |
| 4:D:1:MET:HE2     | 4:D:1:MET:CA      | 2.31                     | 0.57              |
| 4:D:6:ALA:O       | 7:G:5:VAL:HG22    | 2.03                     | 0.57              |
| 7:G:99:VAL:CG2    | 7:G:148:ILE:HD11  | 2.34                     | 0.57              |
| 13:M:249:LEU:HD13 | 14:N:389:PHE:CE1  | 2.38                     | 0.57              |
| 2:B:542:ASN:HD21  | 2:B:587:SER:H     | 1.52                     | 0.57              |
| 2:B:1047:LEU:HD13 | 2:B:1067:ARG:HG2  | 1.86                     | 0.57              |
| 4:D:102:GLU:N     | 4:D:102:GLU:CD    | 2.62                     | 0.57              |
| 13:M:227:CYS:O    | 13:M:229:GLY:N    | 2.37                     | 0.57              |
| 7:G:32:LYS:HZ3    | 7:G:32:LYS:CB     | 2.17                     | 0.57              |
| 2:B:118:GLU:HG3   | 2:B:127:ILE:HG12  | 1.87                     | 0.57              |
| 7:G:122:GLU:OE2   | 7:G:129:TRP:NE1   | 2.37                     | 0.57              |
| 15:O:419:ARG:HD2  | 15:O:422:TYR:CE2  | 2.39                     | 0.57              |
| 3:C:158:ASP:OD1   | 3:C:158:ASP:N     | 2.38                     | 0.57              |
| 10:J:21:TYR:HB2   | 10:J:38:LEU:HD11  | 1.86                     | 0.57              |
| 1:A:93:PHE:H      | 1:A:314:GLN:HE22  | 1.51                     | 0.57              |
| 1:A:328:ILE:H     | 1:A:328:ILE:CD1   | 2.16                     | 0.57              |
| 12:L:19:CYS:HB3   | 12:L:36:CYS:SG    | 2.45                     | 0.57              |
| 1:A:484:ARG:O     | 1:A:484:ARG:HG2   | 2.05                     | 0.56              |
| 1:A:38:SER:HB2    | 1:A:54:GLY:CA     | 2.35                     | 0.56              |
| 1:A:57:ASP:C      | 1:A:59:ARG:N      | 2.63                     | 0.56              |
| 4:D:78:LEU:HD13   | 4:D:86:LEU:HD11   | 1.86                     | 0.56              |
| 15:O:445:ASN:ND2  | 16:P:304:PRO:CG   | 2.59                     | 0.56              |
| 1:A:39:LYS:HB2    | 1:A:41:LEU:H      | 1.71                     | 0.56              |
| 1:A:1113:ILE:HB   | 1:A:1137:ILE:HD11 | 1.87                     | 0.56              |
| 5:E:84:ILE:HG13   | 5:E:114:ALA:HA    | 1.88                     | 0.56              |
| 10:J:53:VAL:O     | 10:J:53:VAL:HG13  | 2.05                     | 0.56              |
| 11:K:35:THR:O     | 11:K:35:THR:HG22  | 2.06                     | 0.56              |
| 1:A:91:PRO:HB3    | 1:A:251:ILE:HD11  | 1.87                     | 0.56              |
| 15:O:113:ASN:HB2  | 15:O:116:LEU:HD21 | 1.86                     | 0.56              |
| 1:A:328:ILE:HD12  | 1:A:328:ILE:N     | 2.21                     | 0.56              |
| 1:A:1124:ASP:HA   | 9:I:21:HIS:CE1    | 2.41                     | 0.56              |
| 3:C:162:LEU:HD23  | 3:C:162:LEU:O     | 2.05                     | 0.56              |
| 15:O:409:ILE:CG1  | 15:O:423:LEU:CD1  | 2.47                     | 0.56              |
| 1:A:1217:GLN:OE1  | 1:A:1217:GLN:N    | 2.38                     | 0.56              |
| 4:D:100:MET:SD    | 7:G:147:GLU:OE1   | 2.64                     | 0.56              |
| 6:F:83:LEU:N      | 6:F:83:LEU:HD23   | 2.21                     | 0.56              |
| 16:P:309:TYR:OH   | 17:Q:32:LEU:O     | 2.24                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:3:LEU:HB3     | 14:N:143:GLU:HG3  | 1.88                     | 0.56              |
| 11:K:60:MET:O     | 11:K:60:MET:HG3   | 2.06                     | 0.56              |
| 19:X:43:DC:H2'    | 19:X:44:DT:C7     | 2.36                     | 0.56              |
| 1:A:1119:GLU:CD   | 1:A:1119:GLU:N    | 2.63                     | 0.56              |
| 2:B:597:ILE:HG13  | 2:B:659:ILE:HG12  | 1.88                     | 0.56              |
| 17:Q:27:LEU:O     | 17:Q:28:PRO:C     | 2.48                     | 0.56              |
| 1:A:41:LEU:HG     | 17:Q:21:PHE:HB3   | 1.89                     | 0.55              |
| 2:B:259:GLU:CD    | 2:B:259:GLU:N     | 2.64                     | 0.55              |
| 3:C:121:LEU:HD13  | 3:C:185:PHE:HE1   | 1.70                     | 0.55              |
| 1:A:180:LYS:NZ    | 1:A:182:ASN:CG    | 2.64                     | 0.55              |
| 2:B:508:ASP:HA    | 2:B:511:ILE:HD12  | 1.88                     | 0.55              |
| 15:O:374:HIS:HB3  | 15:O:423:LEU:HD13 | 1.79                     | 0.55              |
| 1:A:1048:MET:HA   | 1:A:1280:MET:HE1  | 1.88                     | 0.55              |
| 2:B:30:LEU:HD22   | 2:B:663:THR:HG22  | 1.89                     | 0.55              |
| 2:B:294:GLN:NE2   | 19:X:24:DT:H4'    | 2.22                     | 0.55              |
| 9:I:105:ARG:NH2   | 9:I:106:TRP:O     | 2.39                     | 0.55              |
| 20:Y:9:DA:H2''    | 20:Y:10:DG:H5'    | 1.89                     | 0.55              |
| 20:Y:12:DC:C2'    | 20:Y:13:DT:H71    | 2.36                     | 0.55              |
| 1:A:1235:VAL:HG12 | 1:A:1235:VAL:O    | 2.06                     | 0.55              |
| 1:A:335:LYS:HD3   | 1:A:335:LYS:N     | 2.21                     | 0.55              |
| 1:A:1009:THR:O    | 1:A:1012:GLU:HG3  | 2.06                     | 0.55              |
| 1:A:1224:LYS:O    | 1:A:1224:LYS:HG3  | 2.06                     | 0.55              |
| 5:E:46:ASP:HB3    | 5:E:48:PRO:HD2    | 1.87                     | 0.55              |
| 15:O:265:GLU:OE1  | 15:O:268:ARG:NH1  | 2.39                     | 0.55              |
| 1:A:7:ARG:HG3     | 7:G:34:LEU:CD1    | 2.37                     | 0.55              |
| 1:A:370:SER:O     | 1:A:487:ARG:HA    | 2.06                     | 0.55              |
| 1:A:529:LEU:HD23  | 1:A:539:ILE:HD12  | 1.88                     | 0.55              |
| 1:A:1061:MET:CG   | 1:A:1061:MET:O    | 2.55                     | 0.55              |
| 2:B:303:LYS:HA    | 2:B:303:LYS:HE2   | 1.89                     | 0.55              |
| 18:R:11:G:H1      | 20:Y:17:DC:N4     | 1.96                     | 0.55              |
| 2:B:249:GLN:NE2   | 14:N:144:LYS:HE3  | 2.15                     | 0.55              |
| 15:O:99:TYR:OH    | 15:O:150:ARG:NH1  | 2.40                     | 0.55              |
| 1:A:622:LYS:HD3   | 1:A:651:ASP:OD1   | 2.06                     | 0.55              |
| 1:A:1357:THR:OG1  | 2:B:1061:SER:OG   | 2.22                     | 0.55              |
| 4:D:42:LEU:HG     | 7:G:31:ASN:HB3    | 1.87                     | 0.55              |
| 4:D:57:PRO:C      | 4:D:59:ARG:N      | 2.64                     | 0.55              |
| 1:A:1124:ASP:HA   | 9:I:21:HIS:ND1    | 2.22                     | 0.55              |
| 1:A:1232:LEU:HD13 | 1:A:1248:SER:HB2  | 1.89                     | 0.55              |
| 2:B:725:ILE:HG23  | 2:B:730:PHE:HB3   | 1.89                     | 0.55              |
| 4:D:107:ARG:NH2   | 17:Q:82:GLN:OE1   | 2.39                     | 0.55              |
| 5:E:111:THR:HG21  | 19:X:44:DT:P      | 2.47                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:O:37:ARG:O    | 15:O:41:HIS:ND1   | 2.39                     | 0.55              |
| 1:A:588:ILE:HB   | 1:A:594:LEU:HB2   | 1.88                     | 0.54              |
| 1:A:1061:MET:O   | 1:A:1061:MET:SD   | 2.65                     | 0.54              |
| 2:B:1062:MET:HE3 | 2:B:1062:MET:HA   | 1.89                     | 0.54              |
| 9:I:3:LEU:HD13   | 14:N:143:GLU:HG3  | 1.89                     | 0.54              |
| 15:O:410:PRO:HB3 | 15:O:422:TYR:CE2  | 2.42                     | 0.54              |
| 16:P:283:VAL:O   | 16:P:283:VAL:HG13 | 2.07                     | 0.54              |
| 16:P:290:CYS:SG  | 23:P:401:SF4:S4   | 3.04                     | 0.54              |
| 1:A:164:GLY:HA3  | 1:A:177:GLU:CG    | 2.37                     | 0.54              |
| 1:A:720:GLY:HA3  | 1:A:759:ILE:HD11  | 1.88                     | 0.54              |
| 1:A:1053:PHE:CG  | 1:A:1053:PHE:O    | 2.60                     | 0.54              |
| 15:O:86:LEU:HD21 | 15:O:443:ILE:HD13 | 1.89                     | 0.54              |
| 15:O:357:ARG:HA  | 16:P:289:LEU:HD13 | 1.89                     | 0.54              |
| 2:B:182:GLU:HG2  | 2:B:457:SER:HA    | 1.89                     | 0.54              |
| 2:B:896:LYS:HD2  | 2:B:1012:LEU:HD12 | 1.89                     | 0.54              |
| 11:K:30:VAL:HG11 | 11:K:35:THR:HG23  | 1.89                     | 0.54              |
| 15:O:412:THR:OG1 | 15:O:420:THR:HG23 | 2.08                     | 0.54              |
| 1:A:39:LYS:HB2   | 1:A:41:LEU:HB2    | 1.90                     | 0.54              |
| 2:B:392:ILE:HD12 | 2:B:392:ILE:O     | 2.08                     | 0.54              |
| 3:C:265:GLN:HG3  | 3:C:272:VAL:HG12  | 1.88                     | 0.54              |
| 15:O:409:ILE:N   | 15:O:410:PRO:CD   | 2.35                     | 0.54              |
| 16:P:202:PRO:O   | 16:P:205:GLN:NE2  | 2.37                     | 0.54              |
| 19:X:26:DT:H4'   | 19:X:26:DT:OP1    | 2.07                     | 0.54              |
| 1:A:501:ASP:HB2  | 2:B:904:LYS:HG3   | 1.90                     | 0.54              |
| 2:B:784:ASN:N    | 2:B:784:ASN:OD1   | 2.38                     | 0.54              |
| 4:D:39:GLN:HG2   | 7:G:32:LYS:CE     | 2.38                     | 0.54              |
| 4:D:112:GLN:O    | 4:D:112:GLN:NE2   | 2.40                     | 0.54              |
| 1:A:544:ASP:HA   | 1:A:547:THR:CG2   | 2.38                     | 0.54              |
| 2:B:213:ARG:HH21 | 2:B:213:ARG:CB    | 2.18                     | 0.54              |
| 2:B:759:LYS:HG3  | 2:B:910:ILE:HG22  | 1.90                     | 0.54              |
| 7:G:154:ASP:OD1  | 7:G:154:ASP:N     | 2.39                     | 0.54              |
| 11:K:27:LEU:HG   | 11:K:43:VAL:HB    | 1.90                     | 0.54              |
| 13:M:245:TYR:CD2 | 14:N:344:VAL:HG21 | 2.43                     | 0.54              |
| 1:A:1088:GLN:HB3 | 1:A:1242:LYS:HG2  | 1.88                     | 0.54              |
| 4:D:39:GLN:HG2   | 7:G:32:LYS:HE2    | 1.90                     | 0.54              |
| 4:D:96:GLU:O     | 4:D:101:VAL:N     | 2.36                     | 0.54              |
| 1:A:1066:GLY:HA2 | 1:A:1278:HIS:CE1  | 2.43                     | 0.54              |
| 2:B:233:ASP:N    | 2:B:233:ASP:OD1   | 2.41                     | 0.54              |
| 3:C:246:GLU:HG2  | 3:C:272:VAL:HG23  | 1.89                     | 0.54              |
| 16:P:227:LYS:O   | 16:P:240:ASN:ND2  | 2.41                     | 0.54              |
| 19:X:43:DC:N4    | 20:Y:0:DA:N1      | 2.56                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1080:CYS:HB3  | 2:B:1083:CYS:SG   | 2.48                     | 0.53              |
| 15:O:407:GLN:O    | 15:O:410:PRO:CG   | 2.56                     | 0.53              |
| 1:A:154:ASN:HB3   | 1:A:162:PHE:CE1   | 2.43                     | 0.53              |
| 1:A:183:LYS:HD3   | 1:A:183:LYS:N     | 2.22                     | 0.53              |
| 1:A:1045:GLY:HA2  | 1:A:1048:MET:HE3  | 1.90                     | 0.53              |
| 1:A:1137:ILE:HD13 | 1:A:1137:ILE:N    | 2.24                     | 0.53              |
| 2:B:526:LEU:HD12  | 2:B:526:LEU:O     | 2.09                     | 0.53              |
| 15:O:239:LEU:HA   | 15:O:242:PHE:HD2  | 1.73                     | 0.53              |
| 7:G:44:LEU:HB3    | 7:G:77:PHE:HB3    | 1.89                     | 0.53              |
| 15:O:419:ARG:HD2  | 15:O:422:TYR:CZ   | 2.44                     | 0.53              |
| 13:M:64:THR:HG21  | 13:M:96:LEU:HD13  | 1.89                     | 0.53              |
| 1:A:987:TYR:OH    | 8:H:102:ASP:N     | 2.41                     | 0.53              |
| 2:B:812:ASP:HB3   | 12:L:15:MET:HG3   | 1.89                     | 0.53              |
| 4:D:35:HIS:HD2    | 7:G:32:LYS:HE3    | 1.73                     | 0.53              |
| 1:A:42:TYR:O      | 1:A:43:SER:HB3    | 2.08                     | 0.53              |
| 1:A:1125:ASP:N    | 9:I:21:HIS:CE1    | 2.66                     | 0.53              |
| 11:K:48:ASP:N     | 11:K:48:ASP:OD1   | 2.40                     | 0.53              |
| 15:O:115:LYS:HE2  | 15:O:160:CYS:HB2  | 1.89                     | 0.53              |
| 19:X:43:DC:H2'    | 19:X:44:DT:H72    | 1.91                     | 0.53              |
| 1:A:7:ARG:HE      | 4:D:1:MET:HG2     | 1.74                     | 0.53              |
| 1:A:15:ILE:HD13   | 2:B:1126:LEU:HD22 | 1.90                     | 0.53              |
| 1:A:1137:ILE:HD12 | 1:A:1142:LEU:HD11 | 1.89                     | 0.53              |
| 2:B:705:ILE:HG22  | 2:B:705:ILE:O     | 2.08                     | 0.53              |
| 4:D:62:SER:HB2    | 4:D:65:ILE:HG23   | 1.90                     | 0.53              |
| 15:O:171:PRO:O    | 15:O:174:PRO:HD2  | 2.07                     | 0.53              |
| 16:P:290:CYS:HB2  | 16:P:293:PHE:HB2  | 1.90                     | 0.53              |
| 1:A:1186:TYR:CG   | 1:A:1186:TYR:O    | 2.62                     | 0.53              |
| 2:B:375:ASP:OD1   | 2:B:375:ASP:C     | 2.52                     | 0.53              |
| 3:C:266:GLU:OE1   | 3:C:266:GLU:N     | 2.35                     | 0.53              |
| 16:P:286:PRO:HG2  | 16:P:313:TRP:CG   | 2.44                     | 0.53              |
| 8:H:96:VAL:HG22   | 8:H:116:VAL:HG22  | 1.91                     | 0.53              |
| 13:M:249:LEU:HD13 | 14:N:389:PHE:HE1  | 1.74                     | 0.53              |
| 15:O:24:ILE:HD11  | 15:O:45:THR:HG21  | 1.90                     | 0.53              |
| 1:A:37:VAL:O      | 1:A:37:VAL:HG22   | 2.08                     | 0.52              |
| 1:A:547:THR:HG21  | 2:B:932:HIS:NE2   | 2.24                     | 0.52              |
| 1:A:882:LEU:HB2   | 1:A:1034:GLY:HA3  | 1.91                     | 0.52              |
| 1:A:952:ILE:HA    | 1:A:955:LYS:HD3   | 1.90                     | 0.52              |
| 4:D:14:TYR:CE2    | 4:D:18:GLN:HG2    | 2.44                     | 0.52              |
| 4:D:42:LEU:HD13   | 4:D:42:LEU:C      | 2.35                     | 0.52              |
| 1:A:1027:MET:HE2  | 1:A:1031:SER:HB2  | 1.90                     | 0.52              |
| 1:A:1212:ILE:HD11 | 1:A:1223:TYR:HD2  | 1.74                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:32:LYS:CB     | 7:G:32:LYS:NZ     | 2.72                     | 0.52              |
| 15:O:409:ILE:CG1  | 15:O:423:LEU:CG   | 2.84                     | 0.52              |
| 1:A:51:LEU:HG     | 1:A:58:HIS:CD2    | 2.45                     | 0.52              |
| 2:B:384:MET:HG2   | 2:B:402:VAL:HG12  | 1.91                     | 0.52              |
| 4:D:39:GLN:CG     | 7:G:32:LYS:CE     | 2.87                     | 0.52              |
| 13:M:33:ARG:HD2   | 13:M:37:MET:HB2   | 1.91                     | 0.52              |
| 16:P:286:PRO:HG3  | 17:Q:38:PHE:CD2   | 2.44                     | 0.52              |
| 1:A:51:LEU:HB3    | 1:A:56:LEU:O      | 2.09                     | 0.52              |
| 1:A:886:TYR:HB3   | 6:F:53:THR:HG22   | 1.91                     | 0.52              |
| 1:A:1073:ILE:O    | 1:A:1294:MET:HE1  | 2.10                     | 0.52              |
| 1:A:1161:LYS:N    | 1:A:1162:PRO:HD2  | 2.25                     | 0.52              |
| 3:C:130:GLU:CD    | 3:C:130:GLU:H     | 2.15                     | 0.52              |
| 11:K:47:GLU:OE1   | 11:K:47:GLU:HA    | 2.08                     | 0.52              |
| 1:A:463:ASN:HB2   | 1:A:473:ILE:HG12  | 1.90                     | 0.52              |
| 4:D:4:LYS:HE2     | 4:D:4:LYS:CA      | 2.31                     | 0.52              |
| 4:D:59:ARG:NE     | 4:D:59:ARG:H      | 2.07                     | 0.52              |
| 5:E:77:PRO:HG3    | 5:E:90:TYR:HE2    | 1.74                     | 0.52              |
| 6:F:107:ARG:O     | 6:F:107:ARG:HG3   | 2.09                     | 0.52              |
| 8:H:63:THR:HB     | 8:H:70:LEU:HD13   | 1.91                     | 0.52              |
| 12:L:57:ALA:O     | 12:L:58:ARG:C     | 2.53                     | 0.52              |
| 13:M:11:GLN:HB2   | 14:N:331:ILE:HD12 | 1.92                     | 0.52              |
| 15:O:127:ASP:HB3  | 15:O:128:ARG:HH11 | 1.75                     | 0.52              |
| 1:A:151:ARG:HG3   | 1:A:151:ARG:HH11  | 1.74                     | 0.52              |
| 4:D:48:GLU:OE1    | 7:G:103:PHE:CB    | 2.57                     | 0.52              |
| 4:D:48:GLU:CD     | 7:G:103:PHE:CG    | 2.87                     | 0.52              |
| 15:O:376:GLU:HG3  | 15:O:424:TYR:HB2  | 1.91                     | 0.52              |
| 1:A:1214:ILE:HG13 | 1:A:1214:ILE:O    | 2.09                     | 0.52              |
| 4:D:11:LEU:HD21   | 7:G:3:VAL:CA      | 2.37                     | 0.52              |
| 17:Q:80:GLU:HA    | 17:Q:86:ARG:HD3   | 1.92                     | 0.52              |
| 3:C:263:GLU:HG3   | 3:C:274:ARG:HG2   | 1.92                     | 0.51              |
| 13:M:37:MET:HE3   | 14:N:151:THR:HG21 | 1.92                     | 0.51              |
| 15:O:440:TYR:OH   | 15:O:524:GLU:OE2  | 2.27                     | 0.51              |
| 1:A:1375:ARG:NH1  | 1:A:1376:PRO:O    | 2.43                     | 0.51              |
| 13:M:234:GLU:HA   | 13:M:234:GLU:OE2  | 2.09                     | 0.51              |
| 1:A:834:VAL:O     | 1:A:834:VAL:HG23  | 2.10                     | 0.51              |
| 1:A:1185:MET:HB3  | 9:I:14:VAL:O      | 2.10                     | 0.51              |
| 3:C:287:ILE:HG12  | 3:C:297:VAL:HG21  | 1.91                     | 0.51              |
| 15:O:460:LEU:HB3  | 15:O:499:LEU:HD11 | 1.92                     | 0.51              |
| 2:B:412:THR:OG1   | 2:B:413:ASN:N     | 2.43                     | 0.51              |
| 4:D:48:GLU:OE1    | 7:G:103:PHE:CD2   | 2.63                     | 0.51              |
| 15:O:22:GLU:O     | 15:O:26:VAL:N     | 2.40                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:221:LEU:HD21  | 15:O:400:SER:HA   | 1.92                     | 0.51              |
| 1:A:898:ILE:HG22  | 1:A:899:GLN:HG3   | 1.91                     | 0.51              |
| 1:A:1119:GLU:HA   | 1:A:1128:ILE:HA   | 1.93                     | 0.51              |
| 1:A:1179:GLU:OE2  | 1:A:1179:GLU:HA   | 2.10                     | 0.51              |
| 3:C:103:ASP:OD1   | 3:C:103:ASP:N     | 2.44                     | 0.51              |
| 15:O:5:GLU:HG3    | 15:O:83:LEU:HD11  | 1.93                     | 0.51              |
| 16:P:286:PRO:HA   | 17:Q:38:PHE:HD2   | 1.75                     | 0.51              |
| 1:A:1363:LEU:HD21 | 7:G:56:ASP:HB2    | 1.92                     | 0.51              |
| 2:B:196:LYS:CD    | 20:Y:9:DA:OP1     | 2.59                     | 0.51              |
| 1:A:6:PHE:CE2     | 7:G:157:PHE:HA    | 2.44                     | 0.51              |
| 1:A:398:LYS:O     | 1:A:398:LYS:HG2   | 2.11                     | 0.51              |
| 3:C:135:ILE:HD12  | 3:C:135:ILE:N     | 2.23                     | 0.51              |
| 4:D:105:GLU:CD    | 4:D:105:GLU:H     | 2.19                     | 0.51              |
| 5:E:67:ASP:HB3    | 5:E:70:ASP:HB2    | 1.93                     | 0.51              |
| 6:F:75:MET:CB     | 7:G:15:PRO:HG2    | 2.40                     | 0.51              |
| 12:L:34:ILE:H     | 12:L:34:ILE:CD1   | 2.14                     | 0.51              |
| 14:N:269:LEU:HD12 | 14:N:269:LEU:O    | 2.11                     | 0.51              |
| 15:O:407:GLN:N    | 15:O:407:GLN:CD   | 2.69                     | 0.51              |
| 15:O:409:ILE:CB   | 15:O:423:LEU:CD2  | 2.67                     | 0.51              |
| 1:A:17:HIS:O      | 1:A:17:HIS:CG     | 2.63                     | 0.51              |
| 1:A:1129:LEU:HB2  | 1:A:1175:VAL:HG22 | 1.92                     | 0.51              |
| 5:E:7:THR:HG21    | 5:E:41:LYS:HE3    | 1.93                     | 0.51              |
| 5:E:26:TYR:HB3    | 5:E:61:LEU:HB3    | 1.93                     | 0.51              |
| 15:O:60:HIS:NE2   | 15:O:112:LEU:O    | 2.44                     | 0.51              |
| 1:A:601:PHE:CE2   | 1:A:650:MET:HE3   | 2.46                     | 0.51              |
| 2:B:455:ILE:HD11  | 2:B:496:LEU:HG    | 1.92                     | 0.51              |
| 3:C:51:VAL:HG22   | 3:C:65:MET:HG2    | 1.92                     | 0.51              |
| 4:D:39:GLN:HB2    | 7:G:32:LYS:HG2    | 1.93                     | 0.51              |
| 5:E:79:GLU:OE1    | 5:E:79:GLU:N      | 2.44                     | 0.51              |
| 1:A:151:ARG:HB2   | 1:A:151:ARG:CZ    | 2.41                     | 0.50              |
| 1:A:1363:LEU:HA   | 7:G:57:ALA:O      | 2.11                     | 0.50              |
| 12:L:52:LEU:C     | 12:L:52:LEU:HD23  | 2.37                     | 0.50              |
| 1:A:7:ARG:HG2     | 1:A:7:ARG:HH11    | 1.75                     | 0.50              |
| 1:A:36:VAL:HG21   | 1:A:257:VAL:HG21  | 1.93                     | 0.50              |
| 1:A:469:HIS:CD2   | 1:A:471:LEU:HB2   | 2.46                     | 0.50              |
| 1:A:1260:ILE:HD13 | 5:E:207:ARG:NH1   | 2.25                     | 0.50              |
| 1:A:1357:THR:HG1  | 2:B:1061:SER:HG   | 1.57                     | 0.50              |
| 3:C:286:GLU:OE1   | 3:C:286:GLU:HA    | 2.11                     | 0.50              |
| 3:C:292:LYS:HD2   | 3:C:293:LEU:HD12  | 1.93                     | 0.50              |
| 7:G:99:VAL:HG11   | 7:G:148:ILE:HG12  | 1.92                     | 0.50              |
| 8:H:32:SER:OG     | 8:H:35:PHE:O      | 2.27                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1112:GLU:OE1  | 9:I:47:LYS:CE     | 2.58                     | 0.50              |
| 1:A:1225:LEU:HD12 | 1:A:1225:LEU:O    | 2.11                     | 0.50              |
| 2:B:135:ARG:H     | 2:B:412:THR:HG22  | 1.75                     | 0.50              |
| 7:G:148:ILE:CG2   | 7:G:190:ILE:HG23  | 2.29                     | 0.50              |
| 20:Y:2:DC:H2"     | 20:Y:3:DG:C8      | 2.46                     | 0.50              |
| 1:A:7:ARG:HG2     | 1:A:7:ARG:NH1     | 2.27                     | 0.50              |
| 1:A:583:LEU:HD23  | 1:A:583:LEU:H     | 1.76                     | 0.50              |
| 1:A:1360:PHE:O    | 1:A:1360:PHE:CD1  | 2.64                     | 0.50              |
| 2:B:306:ILE:HD13  | 2:B:306:ILE:N     | 2.17                     | 0.50              |
| 3:C:263:GLU:HG3   | 3:C:263:GLU:O     | 2.10                     | 0.50              |
| 7:G:39:VAL:HB     | 7:G:42:VAL:HB     | 1.93                     | 0.50              |
| 16:P:296:CYS:SG   | 16:P:297:HIS:N    | 2.79                     | 0.50              |
| 1:A:424:ARG:HE    | 1:A:447:GLY:HA3   | 1.75                     | 0.50              |
| 1:A:1368:ARG:HB3  | 7:G:22:LEU:HB2    | 1.93                     | 0.50              |
| 2:B:307:GLU:O     | 2:B:311:GLU:HG2   | 2.11                     | 0.50              |
| 2:B:724:THR:HA    | 2:B:727:LEU:HD12  | 1.93                     | 0.50              |
| 4:D:1:MET:SD      | 7:G:7:MET:HE3     | 2.51                     | 0.50              |
| 4:D:102:GLU:N     | 4:D:102:GLU:OE2   | 2.40                     | 0.50              |
| 18:R:11:G:H8      | 18:R:11:G:O5'     | 1.94                     | 0.50              |
| 5:E:47:LYS:C      | 5:E:47:LYS:HD2    | 2.37                     | 0.50              |
| 16:P:286:PRO:HG2  | 16:P:313:TRP:CD2  | 2.47                     | 0.50              |
| 18:R:11:G:O5'     | 18:R:11:G:C8      | 2.65                     | 0.50              |
| 1:A:1239:HIS:HE1  | 5:E:8:TYR:CZ      | 2.29                     | 0.50              |
| 3:C:163:TYR:HE1   | 3:C:204:PRO:HG3   | 1.76                     | 0.50              |
| 4:D:2:GLU:OE1     | 4:D:2:GLU:N       | 2.27                     | 0.50              |
| 4:D:85:GLN:HG2    | 7:G:80:PHE:HZ     | 1.77                     | 0.50              |
| 1:A:16:SER:HB3    | 2:B:1127:LYS:HD2  | 1.94                     | 0.50              |
| 1:A:596:THR:CG2   | 8:H:119:GLY:O     | 2.44                     | 0.50              |
| 1:A:645:LEU:HD22  | 1:A:650:MET:HE2   | 1.93                     | 0.50              |
| 1:A:897:ILE:O     | 1:A:897:ILE:HG22  | 2.12                     | 0.50              |
| 2:B:133:ILE:CG2   | 2:B:133:ILE:O     | 2.60                     | 0.50              |
| 5:E:84:ILE:HG22   | 5:E:88:LYS:HG2    | 1.94                     | 0.50              |
| 7:G:115:GLN:NE2   | 7:G:192:GLU:O     | 2.45                     | 0.50              |
| 1:A:180:LYS:HZ3   | 1:A:182:ASN:CG    | 2.11                     | 0.50              |
| 1:A:211:LEU:HD12  | 1:A:211:LEU:C     | 2.36                     | 0.50              |
| 2:B:555:LEU:C     | 2:B:555:LEU:HD23  | 2.36                     | 0.50              |
| 13:M:7:ASP:OD1    | 13:M:7:ASP:N      | 2.32                     | 0.50              |
| 15:O:436:LEU:HB2  | 15:O:523:LEU:HD22 | 1.92                     | 0.50              |
| 1:A:49:ALA:N      | 1:A:50:PRO:HD3    | 2.26                     | 0.49              |
| 1:A:136:TYR:HE1   | 1:A:140:ARG:HE    | 1.59                     | 0.49              |
| 1:A:1194:GLU:OE1  | 1:A:1194:GLU:HA   | 2.10                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:52:LEU:HD23  | 12:L:52:LEU:O     | 2.12                     | 0.49              |
| 13:M:63:ASP:OD1   | 13:M:63:ASP:N     | 2.45                     | 0.49              |
| 15:O:405:SER:HB3  | 15:O:425:THR:O    | 2.12                     | 0.49              |
| 15:O:450:ARG:O    | 15:O:454:THR:OG1  | 2.29                     | 0.49              |
| 15:O:378:LYS:HD2  | 15:O:379:GLN:HE21 | 1.77                     | 0.49              |
| 1:A:136:TYR:O     | 1:A:136:TYR:CD1   | 2.63                     | 0.49              |
| 1:A:345:LEU:HD11  | 2:B:1120:MET:HE1  | 1.93                     | 0.49              |
| 1:A:727:TYR:CG    | 1:A:751:LEU:HD21  | 2.48                     | 0.49              |
| 1:A:801:GLN:HA    | 1:A:833:PHE:HA    | 1.95                     | 0.49              |
| 1:A:1185:MET:SD   | 1:A:1185:MET:N    | 2.86                     | 0.49              |
| 2:B:721:LYS:HZ3   | 2:B:731:GLU:CD    | 2.19                     | 0.49              |
| 15:O:118:MET:SD   | 17:Q:108:ARG:NH2  | 2.74                     | 0.49              |
| 1:A:958:PHE:HB3   | 1:A:966:LEU:HD11  | 1.95                     | 0.49              |
| 2:B:409:ASP:N     | 2:B:409:ASP:OD1   | 2.43                     | 0.49              |
| 2:B:594:ARG:NH2   | 2:B:663:THR:OG1   | 2.45                     | 0.49              |
| 5:E:47:LYS:N      | 5:E:48:PRO:CD     | 2.76                     | 0.49              |
| 5:E:76:PHE:CD1    | 5:E:76:PHE:N      | 2.80                     | 0.49              |
| 16:P:222:GLU:O    | 16:P:226:SER:OG   | 2.27                     | 0.49              |
| 1:A:164:GLY:HA3   | 1:A:177:GLU:HG3   | 1.95                     | 0.49              |
| 1:A:232:ALA:HB2   | 15:O:6:ILE:CD1    | 2.42                     | 0.49              |
| 1:A:1089:LEU:HD21 | 1:A:1225:LEU:HD21 | 1.95                     | 0.49              |
| 2:B:567:TYR:HB3   | 13:M:250:MET:HG2  | 1.94                     | 0.49              |
| 10:J:40:LEU:HD22  | 10:J:45:CYS:HB3   | 1.94                     | 0.49              |
| 15:O:410:PRO:HB3  | 15:O:422:TYR:CD2  | 2.47                     | 0.49              |
| 15:O:460:LEU:HA   | 15:O:463:LYS:HG2  | 1.94                     | 0.49              |
| 16:P:252:ILE:HG23 | 16:P:257:GLU:HB3  | 1.93                     | 0.49              |
| 17:Q:27:LEU:CD2   | 17:Q:27:LEU:N     | 2.63                     | 0.49              |
| 1:A:183:LYS:H     | 1:A:183:LYS:HE2   | 1.77                     | 0.49              |
| 1:A:1048:MET:HE2  | 1:A:1280:MET:SD   | 2.53                     | 0.49              |
| 17:Q:72:PRO:HA    | 17:Q:75:ILE:HG22  | 1.95                     | 0.49              |
| 2:B:715:PRO:HB2   | 2:B:734:PRO:HG2   | 1.95                     | 0.49              |
| 15:O:409:ILE:CD1  | 15:O:423:LEU:CD1  | 2.63                     | 0.49              |
| 1:A:91:PRO:HG2    | 1:A:221:LEU:HD13  | 1.95                     | 0.49              |
| 1:A:143:LYS:HB2   | 1:A:239:LEU:HD13  | 1.95                     | 0.49              |
| 1:A:442:GLN:HA    | 1:A:442:GLN:NE2   | 2.26                     | 0.49              |
| 1:A:776:SER:N     | 1:A:777:PRO:HD2   | 2.28                     | 0.49              |
| 1:A:1236:MET:HE3  | 1:A:1246:THR:HG22 | 1.94                     | 0.49              |
| 2:B:65:VAL:HG23   | 2:B:75:LEU:O      | 2.13                     | 0.49              |
| 16:P:308:ILE:HD13 | 17:Q:31:VAL:HG11  | 1.93                     | 0.49              |
| 1:A:1369:ASP:OD1  | 1:A:1369:ASP:N    | 2.45                     | 0.49              |
| 3:C:57:ASP:C      | 3:C:57:ASP:OD1    | 2.56                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:52:ARG:N      | 5:E:53:PRO:HD2    | 2.27                     | 0.49              |
| 11:K:58:MET:HE3   | 11:K:58:MET:CA    | 2.42                     | 0.49              |
| 15:O:416:ALA:HA   | 15:O:422:TYR:OH   | 2.13                     | 0.49              |
| 1:A:1346:CYS:HB3  | 1:A:1351:ILE:O    | 2.13                     | 0.48              |
| 7:G:161:SER:HB2   | 7:G:162:PRO:CD    | 2.43                     | 0.48              |
| 1:A:534:ASN:HB2   | 1:A:536:GLU:HG3   | 1.94                     | 0.48              |
| 1:A:1204:ILE:HD12 | 1:A:1204:ILE:N    | 2.28                     | 0.48              |
| 2:B:139:MET:SD    | 2:B:167:GLY:HA2   | 2.53                     | 0.48              |
| 2:B:1080:CYS:CB   | 2:B:1083:CYS:SG   | 3.01                     | 0.48              |
| 15:O:400:SER:OG   | 15:O:401:GLU:OE1  | 2.31                     | 0.48              |
| 20:Y:-1:DC:H2''   | 20:Y:0:DA:C8      | 2.47                     | 0.48              |
| 1:A:571:ILE:HD11  | 1:A:686:LEU:HB2   | 1.94                     | 0.48              |
| 1:A:882:LEU:HD11  | 1:A:1293:LEU:HD12 | 1.96                     | 0.48              |
| 1:A:1140:LEU:HD22 | 9:I:52:VAL:CG1    | 2.41                     | 0.48              |
| 1:A:1233:ARG:CD   | 5:E:134:GLU:HG2   | 2.40                     | 0.48              |
| 12:L:37:ARG:O     | 12:L:38:GLU:HB2   | 2.13                     | 0.48              |
| 14:N:269:LEU:HB3  | 14:N:383:LEU:HB2  | 1.95                     | 0.48              |
| 19:X:37:DG:H2'    | 19:X:38:DA:H8     | 1.76                     | 0.48              |
| 1:A:55:VAL:O      | 1:A:60:MET:HE1    | 2.14                     | 0.48              |
| 1:A:1139:LEU:HD11 | 9:I:53:LEU:HD21   | 1.94                     | 0.48              |
| 11:K:58:MET:HE2   | 11:K:102:GLU:HB3  | 1.94                     | 0.48              |
| 16:P:219:TYR:HD2  | 16:P:271:ARG:HB3  | 1.78                     | 0.48              |
| 16:P:286:PRO:HA   | 17:Q:38:PHE:CD2   | 2.48                     | 0.48              |
| 19:X:38:DA:H61    | 20:Y:6:DT:H3      | 1.60                     | 0.48              |
| 1:A:1048:MET:CG   | 1:A:1280:MET:HE1  | 2.43                     | 0.48              |
| 1:A:1269:ASN:O    | 1:A:1273:TYR:N    | 2.43                     | 0.48              |
| 3:C:43:ASP:OD1    | 3:C:43:ASP:N      | 2.46                     | 0.48              |
| 1:A:1297:LYS:HB3  | 1:A:1301:LEU:HD11 | 1.96                     | 0.48              |
| 1:A:1347:ILE:HD13 | 2:B:1052:ARG:HD2  | 1.96                     | 0.48              |
| 2:B:253:GLN:HG3   | 14:N:146:GLU:OE2  | 2.14                     | 0.48              |
| 2:B:672:ILE:HG12  | 2:B:686:GLN:HG3   | 1.94                     | 0.48              |
| 3:C:210:LEU:C     | 3:C:210:LEU:HD12  | 2.39                     | 0.48              |
| 4:D:61:GLN:HA     | 4:D:61:GLN:NE2    | 2.28                     | 0.48              |
| 7:G:84:ILE:HD11   | 7:G:149:ARG:HH21  | 1.77                     | 0.48              |
| 15:O:445:ASN:CG   | 23:P:401:SF4:S2   | 2.97                     | 0.48              |
| 1:A:213:ARG:H     | 1:A:213:ARG:CD    | 2.27                     | 0.48              |
| 1:A:331:ASN:ND2   | 1:A:331:ASN:C     | 2.68                     | 0.48              |
| 1:A:385:HIS:HB2   | 2:B:1020:MET:HE1  | 1.95                     | 0.48              |
| 2:B:75:LEU:HD13   | 2:B:119:TYR:HB3   | 1.95                     | 0.48              |
| 2:B:781:ARG:NH2   | 2:B:781:ARG:HB3   | 2.29                     | 0.48              |
| 3:C:332:LYS:HB3   | 11:K:51:LEU:HD22  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:11:LEU:HD22   | 7:G:4:LEU:HD22    | 1.96                     | 0.48              |
| 4:D:43:ASN:HD22   | 4:D:43:ASN:N      | 2.01                     | 0.48              |
| 6:F:126:THR:O     | 6:F:126:THR:OG1   | 2.23                     | 0.48              |
| 16:P:220:ILE:CD1  | 16:P:271:ARG:HD2  | 2.43                     | 0.48              |
| 17:Q:57:MET:O     | 17:Q:61:LYS:N     | 2.38                     | 0.48              |
| 1:A:587:THR:HG23  | 1:A:599:GLN:OE1   | 2.12                     | 0.48              |
| 1:A:1033:VAL:HG13 | 1:A:1289:LEU:HD22 | 1.95                     | 0.48              |
| 1:A:1239:HIS:CE1  | 5:E:8:TYR:CZ      | 3.02                     | 0.48              |
| 2:B:184:LEU:HD23  | 2:B:190:ILE:HD13  | 1.96                     | 0.48              |
| 2:B:303:LYS:HE2   | 2:B:303:LYS:CA    | 2.44                     | 0.48              |
| 2:B:530:GLU:OE1   | 2:B:530:GLU:N     | 2.46                     | 0.48              |
| 3:C:23:ASN:O      | 3:C:303:ARG:NH2   | 2.47                     | 0.48              |
| 3:C:97:ASN:C      | 3:C:97:ASN:OD1    | 2.55                     | 0.48              |
| 3:C:264:VAL:HG23  | 3:C:264:VAL:O     | 2.13                     | 0.48              |
| 3:C:319:ASP:OD1   | 3:C:319:ASP:N     | 2.44                     | 0.48              |
| 20:Y:2:DC:C5      | 20:Y:2:DC:OP2     | 2.66                     | 0.48              |
| 2:B:196:LYS:HD2   | 20:Y:9:DA:OP1     | 2.14                     | 0.48              |
| 7:G:151:ARG:NH1   | 7:G:152:VAL:HG12  | 2.29                     | 0.48              |
| 8:H:76:ASN:ND2    | 11:K:87:ARG:NE    | 2.53                     | 0.48              |
| 20:Y:4:DG:H2'     | 20:Y:5:DC:C6      | 2.48                     | 0.48              |
| 1:A:1239:HIS:HE1  | 5:E:8:TYR:CE1     | 2.32                     | 0.47              |
| 4:D:52:TYR:O      | 4:D:55:LYS:HB2    | 2.14                     | 0.47              |
| 5:E:82:VAL:HG13   | 5:E:86:THR:HB     | 1.96                     | 0.47              |
| 7:G:161:SER:HB2   | 7:G:162:PRO:HD3   | 1.96                     | 0.47              |
| 11:K:37:ARG:HB3   | 11:K:91:PRO:HA    | 1.95                     | 0.47              |
| 11:K:89:THR:HG22  | 11:K:89:THR:O     | 2.14                     | 0.47              |
| 1:A:386:VAL:HG22  | 2:B:1022:ALA:HB2  | 1.96                     | 0.47              |
| 1:A:474:MET:HE2   | 1:A:525:THR:HG22  | 1.95                     | 0.47              |
| 1:A:574:GLY:O     | 1:A:575:LYS:HB3   | 2.13                     | 0.47              |
| 2:B:40:VAL:HG12   | 2:B:40:VAL:O      | 2.14                     | 0.47              |
| 2:B:505:ASP:OD1   | 2:B:505:ASP:N     | 2.44                     | 0.47              |
| 2:B:551:ASP:O     | 2:B:551:ASP:CG    | 2.56                     | 0.47              |
| 15:O:84:ARG:NH2   | 15:O:524:GLU:OE1  | 2.46                     | 0.47              |
| 15:O:414:ASP:OD1  | 15:O:414:ASP:N    | 2.44                     | 0.47              |
| 1:A:35:GLN:HG2    | 1:A:37:VAL:HB     | 1.97                     | 0.47              |
| 1:A:1065:LEU:O    | 1:A:1274:THR:OG1  | 2.33                     | 0.47              |
| 1:A:1261:GLU:CG   | 5:E:193:ILE:HD13  | 2.40                     | 0.47              |
| 9:I:8:CYS:HB2     | 13:M:139:PHE:HE1  | 1.79                     | 0.47              |
| 1:A:183:LYS:H     | 1:A:183:LYS:CE    | 2.28                     | 0.47              |
| 1:A:1295:THR:O    | 1:A:1295:THR:OG1  | 2.27                     | 0.47              |
| 2:B:242:ALA:HB1   | 2:B:284:LEU:CD2   | 2.44                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:514:LEU:HD22 | 2:B:568:ILE:HD11  | 1.95                     | 0.47              |
| 2:B:686:GLN:HA   | 2:B:686:GLN:NE2   | 2.29                     | 0.47              |
| 9:I:44:PRO:O     | 9:I:86:SER:OG     | 2.32                     | 0.47              |
| 1:A:563:LYS:O    | 1:A:567:ILE:HG12  | 2.15                     | 0.47              |
| 2:B:106:ASP:HA   | 2:B:173:GLY:HA3   | 1.97                     | 0.47              |
| 9:I:1:MET:HE1    | 14:N:153:GLN:OE1  | 2.15                     | 0.47              |
| 12:L:25:GLU:CD   | 12:L:25:GLU:N     | 2.69                     | 0.47              |
| 19:X:43:DC:H42   | 20:Y:1:DG:H1      | 1.61                     | 0.47              |
| 1:A:34:ILE:HD12  | 1:A:34:ILE:HA     | 1.71                     | 0.47              |
| 1:A:197:PHE:O    | 1:A:197:PHE:CD1   | 2.64                     | 0.47              |
| 1:A:205:LYS:NZ   | 1:A:205:LYS:HB3   | 2.29                     | 0.47              |
| 1:A:630:ASP:OD1  | 1:A:630:ASP:N     | 2.47                     | 0.47              |
| 1:A:868:THR:HG21 | 1:A:1046:THR:HG22 | 1.96                     | 0.47              |
| 2:B:562:MET:CE   | 13:M:250:MET:HE3  | 2.44                     | 0.47              |
| 2:B:1053:ASP:HA  | 2:B:1056:ILE:HD12 | 1.96                     | 0.47              |
| 6:F:107:ARG:HD3  | 6:F:115:TYR:HB2   | 1.97                     | 0.47              |
| 15:O:20:ILE:HD11 | 17:Q:68:MET:HG3   | 1.95                     | 0.47              |
| 15:O:156:PHE:HA  | 15:O:241:ARG:HG2  | 1.96                     | 0.47              |
| 15:O:412:THR:CG2 | 15:O:413:PRO:HD2  | 2.45                     | 0.47              |
| 1:A:196:SER:HB2  | 15:O:373:LYS:CE   | 2.40                     | 0.47              |
| 1:A:941:SER:CB   | 1:A:980:ILE:HG21  | 2.42                     | 0.47              |
| 1:A:1048:MET:CA  | 1:A:1280:MET:HE1  | 2.44                     | 0.47              |
| 1:A:1112:GLU:HB3 | 9:I:47:LYS:HG2    | 1.95                     | 0.47              |
| 1:A:1192:LEU:O   | 1:A:1196:LEU:N    | 2.47                     | 0.47              |
| 2:B:424:TRP:HB2  | 2:B:436:VAL:HG21  | 1.96                     | 0.47              |
| 4:D:43:ASN:ND2   | 4:D:43:ASN:N      | 2.57                     | 0.47              |
| 6:F:78:PRO:HD2   | 7:G:18:PHE:HB2    | 1.96                     | 0.47              |
| 7:G:160:THR:O    | 7:G:160:THR:CG2   | 2.63                     | 0.47              |
| 13:M:59:GLU:HG2  | 13:M:101:THR:HG22 | 1.96                     | 0.47              |
| 15:O:357:ARG:HA  | 16:P:289:LEU:CD1  | 2.44                     | 0.47              |
| 16:P:283:VAL:O   | 16:P:283:VAL:CG1  | 2.62                     | 0.47              |
| 1:A:104:ILE:HG23 | 1:A:238:LEU:HD22  | 1.96                     | 0.47              |
| 1:A:210:LEU:HB3  | 15:O:411:LYS:HD2  | 1.96                     | 0.47              |
| 1:A:427:GLN:N    | 1:A:427:GLN:CD    | 2.73                     | 0.47              |
| 1:A:1235:VAL:O   | 1:A:1241:VAL:HG11 | 2.14                     | 0.47              |
| 2:B:828:VAL:HG22 | 2:B:856:ILE:HB    | 1.97                     | 0.47              |
| 4:D:1:MET:HE1    | 7:G:7:MET:HE3     | 1.96                     | 0.47              |
| 15:O:406:LEU:N   | 15:O:406:LEU:HD23 | 2.30                     | 0.47              |
| 1:A:149:LYS:O    | 1:A:152:LYS:HB2   | 2.15                     | 0.47              |
| 1:A:322:ASN:HD22 | 1:A:323:SER:N     | 2.13                     | 0.47              |
| 1:A:954:LYS:NZ   | 1:A:954:LYS:HB2   | 2.30                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:55:ARG:N      | 5:E:55:ARG:CD     | 2.77                     | 0.47              |
| 10:J:16:ASN:OD1   | 10:J:16:ASN:N     | 2.47                     | 0.47              |
| 13:M:245:TYR:HD2  | 14:N:344:VAL:HG21 | 1.80                     | 0.47              |
| 17:Q:86:ARG:HB2   | 17:Q:86:ARG:HH11  | 1.80                     | 0.47              |
| 1:A:703:VAL:HG13  | 1:A:795:MET:HB3   | 1.97                     | 0.47              |
| 4:D:48:GLU:OE1    | 7:G:103:PHE:HB3   | 2.15                     | 0.47              |
| 5:E:61:LEU:N      | 5:E:61:LEU:HD13   | 2.30                     | 0.46              |
| 6:F:115:TYR:CD1   | 6:F:115:TYR:C     | 2.92                     | 0.46              |
| 16:P:308:ILE:HD13 | 17:Q:31:VAL:CG1   | 2.45                     | 0.46              |
| 1:A:291:ASP:HB2   | 17:Q:23:LYS:HE2   | 1.97                     | 0.46              |
| 2:B:757:LEU:HD23  | 2:B:762:LEU:HD21  | 1.97                     | 0.46              |
| 2:B:920:ASP:OD2   | 3:C:301:ARG:NH2   | 2.47                     | 0.46              |
| 3:C:65:MET:HE2    | 3:C:68:ILE:CG2    | 2.43                     | 0.46              |
| 3:C:203:ARG:HB3   | 3:C:204:PRO:HD2   | 1.97                     | 0.46              |
| 4:D:1:MET:O       | 4:D:1:MET:HG3     | 2.15                     | 0.46              |
| 1:A:1034:GLY:HA2  | 1:A:1289:LEU:HD21 | 1.97                     | 0.46              |
| 1:A:1215:ASP:C    | 1:A:1215:ASP:OD1  | 2.58                     | 0.46              |
| 2:B:384:MET:HE2   | 2:B:384:MET:HB2   | 1.39                     | 0.46              |
| 2:B:733:LEU:N     | 2:B:733:LEU:CD2   | 2.78                     | 0.46              |
| 2:B:973:CYS:HB2   | 2:B:983:TYR:HB2   | 1.97                     | 0.46              |
| 7:G:94:PRO:HA     | 7:G:121:ASP:HB2   | 1.96                     | 0.46              |
| 15:O:26:VAL:HA    | 15:O:29:ILE:HD12  | 1.97                     | 0.46              |
| 16:P:269:LEU:HD23 | 16:P:269:LEU:HA   | 1.78                     | 0.46              |
| 1:A:36:VAL:O      | 1:A:36:VAL:CG1    | 2.62                     | 0.46              |
| 1:A:481:LYS:HB2   | 1:A:487:ARG:HH21  | 1.80                     | 0.46              |
| 2:B:133:ILE:O     | 2:B:133:ILE:HG22  | 2.15                     | 0.46              |
| 2:B:1112:LEU:O    | 2:B:1116:GLU:HG2  | 2.14                     | 0.46              |
| 7:G:79:PRO:HG2    | 7:G:150:PHE:CD2   | 2.51                     | 0.46              |
| 14:N:139:ASN:O    | 14:N:142:LYS:NZ   | 2.42                     | 0.46              |
| 16:P:294:ASP:OD1  | 16:P:294:ASP:C    | 2.58                     | 0.46              |
| 17:Q:81:ARG:HE    | 17:Q:84:ILE:HD11  | 1.81                     | 0.46              |
| 20:Y:3:DG:H2''    | 20:Y:4:DG:O4'     | 2.16                     | 0.46              |
| 1:A:91:PRO:CB     | 1:A:251:ILE:HD11  | 2.45                     | 0.46              |
| 2:B:854:VAL:HG12  | 2:B:854:VAL:O     | 2.16                     | 0.46              |
| 7:G:80:PHE:CE2    | 7:G:82:ASP:HB2    | 2.51                     | 0.46              |
| 10:J:31:GLU:OE1   | 10:J:31:GLU:HA    | 2.15                     | 0.46              |
| 1:A:39:LYS:CA     | 17:Q:24:GLY:HA3   | 2.45                     | 0.46              |
| 1:A:881:ASP:OD1   | 1:A:881:ASP:N     | 2.27                     | 0.46              |
| 1:A:1080:ILE:HD13 | 1:A:1249:ASN:O    | 2.16                     | 0.46              |
| 1:A:1364:HIS:N    | 7:G:57:ALA:O      | 2.49                     | 0.46              |
| 2:B:338:MET:O     | 2:B:342:VAL:HG23  | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:957:ARG:NH1   | 2:B:957:ARG:HB2   | 2.31                     | 0.46              |
| 3:C:29:PHE:HB2    | 3:C:32:ASN:ND2    | 2.30                     | 0.46              |
| 3:C:275:VAL:O     | 3:C:275:VAL:HG23  | 2.16                     | 0.46              |
| 4:D:32:LYS:HD3    | 4:D:32:LYS:H      | 1.80                     | 0.46              |
| 15:O:147:THR:HA   | 15:O:150:ARG:HB2  | 1.98                     | 0.46              |
| 20:Y:9:DA:H2''    | 20:Y:10:DG:C5'    | 2.46                     | 0.46              |
| 1:A:1145:ASN:HB3  | 1:A:1148:THR:HG23 | 1.98                     | 0.46              |
| 15:O:170:ASP:O    | 15:O:173:PRO:HD2  | 2.15                     | 0.46              |
| 15:O:409:ILE:HG22 | 15:O:409:ILE:O    | 2.15                     | 0.46              |
| 20:Y:3:DG:H2'     | 20:Y:4:DG:C8      | 2.50                     | 0.46              |
| 2:B:613:GLU:HA    | 2:B:613:GLU:OE1   | 2.15                     | 0.46              |
| 4:D:84:LEU:O      | 4:D:84:LEU:HD12   | 2.16                     | 0.46              |
| 15:O:19:GLU:OE2   | 17:Q:70:ARG:NE    | 2.47                     | 0.46              |
| 2:B:131:LEU:HD11  | 2:B:403:VAL:HG13  | 1.96                     | 0.46              |
| 2:B:335:THR:O     | 2:B:339:VAL:HG23  | 2.15                     | 0.46              |
| 3:C:155:ASP:N     | 3:C:155:ASP:OD1   | 2.49                     | 0.46              |
| 6:F:75:MET:HB3    | 7:G:15:PRO:HG2    | 1.98                     | 0.46              |
| 11:K:58:MET:HA    | 11:K:58:MET:CE    | 2.46                     | 0.46              |
| 19:X:42:DG:H2''   | 19:X:43:DC:O4'    | 2.15                     | 0.46              |
| 20:Y:11:DT:H2''   | 20:Y:12:DC:C6     | 2.50                     | 0.46              |
| 1:A:105:LEU:HD13  | 1:A:218:LEU:HD13  | 1.98                     | 0.46              |
| 1:A:183:LYS:H     | 1:A:183:LYS:CD    | 2.28                     | 0.46              |
| 2:B:294:GLN:HE21  | 19:X:24:DT:H4'    | 1.80                     | 0.46              |
| 2:B:486:GLU:HG2   | 2:B:486:GLU:O     | 2.15                     | 0.46              |
| 15:O:412:THR:HG22 | 15:O:413:PRO:HD2  | 1.98                     | 0.46              |
| 1:A:115:ILE:CD1   | 1:A:237:LEU:HB3   | 2.46                     | 0.45              |
| 1:A:378:ASP:OD1   | 1:A:379:GLU:HG3   | 2.15                     | 0.45              |
| 2:B:536:VAL:HG13  | 2:B:548:VAL:HG13  | 1.98                     | 0.45              |
| 2:B:542:ASN:ND2   | 2:B:587:SER:H     | 2.13                     | 0.45              |
| 2:B:578:LEU:HD23  | 2:B:578:LEU:N     | 2.25                     | 0.45              |
| 3:C:337:LEU:HD23  | 3:C:337:LEU:HA    | 1.82                     | 0.45              |
| 20:Y:9:DA:H2'     | 20:Y:10:DG:C8     | 2.51                     | 0.45              |
| 1:A:446:TYR:N     | 1:A:446:TYR:CD1   | 2.84                     | 0.45              |
| 1:A:1135:GLU:O    | 1:A:1139:LEU:N    | 2.36                     | 0.45              |
| 1:A:1228:GLU:N    | 1:A:1228:GLU:OE1  | 2.49                     | 0.45              |
| 2:B:520:VAL:HA    | 2:B:549:ILE:HG23  | 1.97                     | 0.45              |
| 15:O:59:GLN:NE2   | 15:O:113:ASN:O    | 2.42                     | 0.45              |
| 1:A:45:ASP:N      | 1:A:50:PRO:O      | 2.43                     | 0.45              |
| 1:A:412:PRO:O     | 1:A:453:HIS:HE1   | 1.98                     | 0.45              |
| 2:B:119:TYR:CD1   | 2:B:119:TYR:N     | 2.84                     | 0.45              |
| 2:B:196:LYS:HD3   | 20:Y:9:DA:P       | 2.56                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:464:LYS:HE3   | 19:X:30:DC:H5"    | 1.98                     | 0.45              |
| 2:B:743:VAL:HG22  | 2:B:743:VAL:O     | 2.16                     | 0.45              |
| 2:B:984:LEU:HD12  | 2:B:984:LEU:HA    | 1.77                     | 0.45              |
| 4:D:85:GLN:NE2    | 7:G:83:GLU:CA     | 2.69                     | 0.45              |
| 11:K:31:GLN:C     | 11:K:31:GLN:CD    | 2.82                     | 0.45              |
| 11:K:38:HIS:CE1   | 11:K:89:THR:HA    | 2.52                     | 0.45              |
| 13:M:67:PRO:HD2   | 14:N:138:ILE:HG12 | 1.97                     | 0.45              |
| 13:M:238:LEU:CD1  | 14:N:341:LEU:HG   | 2.44                     | 0.45              |
| 14:N:261:THR:HG22 | 14:N:263:GLU:H    | 1.82                     | 0.45              |
| 15:O:406:LEU:N    | 15:O:406:LEU:CD2  | 2.79                     | 0.45              |
| 15:O:445:ASN:HD22 | 16:P:304:PRO:CG   | 2.26                     | 0.45              |
| 2:B:65:VAL:HG23   | 2:B:75:LEU:HB3    | 1.98                     | 0.45              |
| 2:B:478:MET:HB3   | 2:B:592:LEU:HD13  | 1.98                     | 0.45              |
| 4:D:7:ASN:ND2     | 17:Q:78:PRO:HG3   | 2.29                     | 0.45              |
| 5:E:21:CYS:SG     | 5:E:61:LEU:HG     | 2.57                     | 0.45              |
| 5:E:61:LEU:H      | 5:E:61:LEU:CD2    | 2.12                     | 0.45              |
| 19:X:40:DC:H6     | 19:X:40:DC:OP2    | 1.99                     | 0.45              |
| 1:A:794:GLN:HG2   | 1:A:799:VAL:HA    | 1.98                     | 0.45              |
| 1:A:1135:GLU:OE1  | 1:A:1135:GLU:HA   | 2.16                     | 0.45              |
| 1:A:1315:VAL:O    | 1:A:1319:ALA:N    | 2.47                     | 0.45              |
| 2:B:189:ILE:H     | 2:B:189:ILE:HG13  | 1.56                     | 0.45              |
| 11:K:27:LEU:HD21  | 11:K:45:HIS:CE1   | 2.52                     | 0.45              |
| 2:B:574:ILE:HD13  | 2:B:574:ILE:N     | 2.31                     | 0.45              |
| 2:B:623:ASP:OD1   | 2:B:623:ASP:N     | 2.50                     | 0.45              |
| 4:D:59:ARG:HB3    | 4:D:59:ARG:NH2    | 2.32                     | 0.45              |
| 10:J:19:GLU:OE1   | 10:J:19:GLU:N     | 2.50                     | 0.45              |
| 10:J:28:GLU:C     | 10:J:28:GLU:CD    | 2.84                     | 0.45              |
| 11:K:94:GLU:HB3   | 11:K:95:PRO:HD3   | 1.98                     | 0.45              |
| 1:A:94:HIS:CD2    | 1:A:96:GLY:H      | 2.34                     | 0.45              |
| 1:A:700:ILE:HD11  | 2:B:944:ILE:HG12  | 1.99                     | 0.45              |
| 1:A:1017:THR:HG22 | 1:A:1021:LYS:HD2  | 1.99                     | 0.45              |
| 1:A:1150:ARG:HD2  | 1:A:1167:VAL:HG13 | 1.98                     | 0.45              |
| 1:A:1328:LEU:HD23 | 1:A:1328:LEU:HA   | 1.83                     | 0.45              |
| 2:B:883:MET:HE2   | 2:B:883:MET:HB2   | 1.66                     | 0.45              |
| 3:C:266:GLU:N     | 3:C:266:GLU:CD    | 2.75                     | 0.45              |
| 3:C:292:LYS:O     | 3:C:292:LYS:HD3   | 2.16                     | 0.45              |
| 7:G:160:THR:O     | 7:G:160:THR:HG22  | 2.15                     | 0.45              |
| 15:O:416:ALA:HB3  | 15:O:417:PRO:HD3  | 1.98                     | 0.45              |
| 15:O:423:LEU:HD23 | 15:O:423:LEU:N    | 2.32                     | 0.45              |
| 1:A:117:LEU:HB3   | 1:A:122:LYS:HG3   | 1.99                     | 0.45              |
| 1:A:575:LYS:O     | 1:A:575:LYS:HG2   | 2.15                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:384:MET:SD    | 2:B:406:MET:HG2   | 2.57                     | 0.45              |
| 15:O:63:VAL:HG22  | 15:O:77:ALA:HB2   | 1.99                     | 0.45              |
| 1:A:176:HIS:CE1   | 1:A:178:LYS:HB2   | 2.52                     | 0.45              |
| 1:A:1074:ILE:CD1  | 1:A:1290:LEU:HD21 | 2.47                     | 0.45              |
| 1:A:1305:ARG:HD2  | 1:A:1323:LYS:HE3  | 1.99                     | 0.45              |
| 2:B:989:VAL:CG2   | 2:B:998:LEU:HD12  | 2.47                     | 0.45              |
| 5:E:46:ASP:C      | 5:E:48:PRO:HD2    | 2.41                     | 0.45              |
| 5:E:82:VAL:O      | 5:E:111:THR:HG22  | 2.17                     | 0.45              |
| 7:G:151:ARG:CZ    | 7:G:152:VAL:HG12  | 2.47                     | 0.45              |
| 20:Y:10:DG:H2''   | 20:Y:11:DT:C5'    | 2.43                     | 0.45              |
| 1:A:7:ARG:HG3     | 7:G:34:LEU:HD13   | 1.97                     | 0.45              |
| 1:A:990:ASN:CG    | 1:A:990:ASN:O     | 2.60                     | 0.45              |
| 1:A:1196:LEU:N    | 1:A:1197:PRO:HD2  | 2.32                     | 0.45              |
| 2:B:570:GLU:H     | 2:B:570:GLU:HG3   | 1.50                     | 0.45              |
| 6:F:69:ARG:HD2    | 6:F:69:ARG:HA     | 1.74                     | 0.45              |
| 9:I:32:HIS:NE2    | 14:N:137:ILE:HG12 | 2.31                     | 0.45              |
| 15:O:447:ILE:O    | 15:O:451:GLN:N    | 2.47                     | 0.45              |
| 15:O:459:ARG:HG2  | 15:O:460:LEU:HD23 | 1.99                     | 0.45              |
| 16:P:293:PHE:CD2  | 23:P:401:SF4:S1   | 3.10                     | 0.45              |
| 1:A:1206:GLU:CD   | 1:A:1231:ASN:HB2  | 2.42                     | 0.44              |
| 2:B:128:ARG:CZ    | 2:B:403:VAL:HG11  | 2.47                     | 0.44              |
| 7:G:161:SER:CB    | 7:G:162:PRO:CD    | 2.95                     | 0.44              |
| 4:D:117:LEU:HA    | 4:D:120:VAL:HG12  | 1.98                     | 0.44              |
| 8:H:38:ASP:OD1    | 8:H:38:ASP:N      | 2.42                     | 0.44              |
| 1:A:99:ARG:HA     | 1:A:102:ILE:HD12  | 2.00                     | 0.44              |
| 1:A:1132:LEU:HD11 | 1:A:1149:VAL:HG21 | 1.99                     | 0.44              |
| 2:B:1062:MET:HE3  | 2:B:1062:MET:CA   | 2.48                     | 0.44              |
| 10:J:33:ASP:OD1   | 10:J:33:ASP:C     | 2.60                     | 0.44              |
| 13:M:50:LYS:HD3   | 13:M:203:GLU:HB3  | 1.98                     | 0.44              |
| 1:A:29:ARG:HD2    | 16:P:301:GLU:OE2  | 2.18                     | 0.44              |
| 2:B:245:VAL:HG22  | 2:B:245:VAL:O     | 2.16                     | 0.44              |
| 3:C:118:ASP:C     | 3:C:118:ASP:OD1   | 2.59                     | 0.44              |
| 3:C:181:GLN:HG2   | 3:C:185:PHE:HE2   | 1.82                     | 0.44              |
| 4:D:58:CYS:CA     | 4:D:61:GLN:HB2    | 2.39                     | 0.44              |
| 1:A:142:LEU:HD23  | 1:A:142:LEU:HA    | 1.76                     | 0.44              |
| 1:A:651:ASP:CG    | 1:A:783:CYS:HA    | 2.41                     | 0.44              |
| 1:A:1239:HIS:CE1  | 5:E:8:TYR:CE2     | 3.06                     | 0.44              |
| 2:B:598:ILE:HD12  | 2:B:628:SER:O     | 2.17                     | 0.44              |
| 3:C:17:GLY:HA3    | 3:C:22:ARG:HH12   | 1.83                     | 0.44              |
| 6:F:107:ARG:NH2   | 7:G:56:ASP:OD2    | 2.41                     | 0.44              |
| 7:G:56:ASP:OD1    | 7:G:56:ASP:N      | 2.41                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:M:240:LYS:NZ   | 13:M:248:MET:SD   | 2.87                     | 0.44              |
| 1:A:44:GLN:OE1    | 1:A:44:GLN:HA     | 2.18                     | 0.44              |
| 1:A:760:ARG:HH22  | 1:A:794:GLN:HG3   | 1.83                     | 0.44              |
| 2:B:446:ILE:H     | 2:B:446:ILE:HG12  | 1.66                     | 0.44              |
| 7:G:26:ILE:HG21   | 7:G:70:VAL:HG21   | 1.98                     | 0.44              |
| 15:O:357:ARG:HD2  | 16:P:288:GLY:O    | 2.16                     | 0.44              |
| 18:R:9:C:H2'      | 18:R:10:U:C6      | 2.52                     | 0.44              |
| 1:A:118:SER:O     | 1:A:122:LYS:N     | 2.42                     | 0.44              |
| 1:A:237:LEU:HD12  | 1:A:237:LEU:HA    | 1.70                     | 0.44              |
| 1:A:410:ASN:HB3   | 1:A:414:VAL:HB    | 1.99                     | 0.44              |
| 1:A:1140:LEU:O    | 1:A:1142:LEU:HD23 | 2.17                     | 0.44              |
| 2:B:59:MET:HE1    | 2:B:79:ASN:N      | 2.33                     | 0.44              |
| 15:O:406:LEU:HD23 | 15:O:406:LEU:H    | 1.83                     | 0.44              |
| 15:O:415:HIS:HB2  | 15:O:418:SER:O    | 2.18                     | 0.44              |
| 16:P:256:LYS:HE2  | 16:P:278:PRO:HA   | 1.99                     | 0.44              |
| 1:A:1161:LYS:N    | 1:A:1161:LYS:HD3  | 2.33                     | 0.44              |
| 1:A:1297:LYS:HE2  | 1:A:1297:LYS:HB2  | 1.87                     | 0.44              |
| 2:B:303:LYS:HA    | 2:B:303:LYS:CE    | 2.48                     | 0.44              |
| 2:B:707:THR:HA    | 2:B:774:ASN:HB3   | 1.99                     | 0.44              |
| 3:C:38:ASP:O      | 11:K:61:LYS:NZ    | 2.51                     | 0.44              |
| 3:C:96:ASN:CG     | 3:C:96:ASN:O      | 2.60                     | 0.44              |
| 11:K:67:PHE:CD1   | 11:K:67:PHE:C     | 2.95                     | 0.44              |
| 15:O:434:MET:HE2  | 15:O:434:MET:HB3  | 1.86                     | 0.44              |
| 17:Q:78:PRO:HD2   | 17:Q:79:GLU:CD    | 2.43                     | 0.44              |
| 2:B:1108:TYR:CD1  | 2:B:1108:TYR:C    | 2.96                     | 0.44              |
| 13:M:66:ASN:HB2   | 14:N:138:ILE:HG13 | 2.00                     | 0.44              |
| 15:O:345:LEU:HD23 | 15:O:345:LEU:HA   | 1.89                     | 0.44              |
| 1:A:229:ARG:HD2   | 15:O:433:ARG:HB3  | 2.00                     | 0.43              |
| 1:A:782:LEU:HD23  | 1:A:789:PHE:HZ    | 1.83                     | 0.43              |
| 1:A:1082:THR:N    | 1:A:1083:PRO:HD3  | 2.33                     | 0.43              |
| 2:B:262:MET:HB3   | 9:I:2:LEU:HD12    | 2.00                     | 0.43              |
| 2:B:1115:GLN:OE1  | 2:B:1115:GLN:CA   | 2.65                     | 0.43              |
| 4:D:100:MET:SD    | 7:G:147:GLU:OE2   | 2.76                     | 0.43              |
| 13:M:6:ASP:OD1    | 13:M:6:ASP:N      | 2.50                     | 0.43              |
| 1:A:516:LYS:HB3   | 1:A:516:LYS:HE2   | 1.64                     | 0.43              |
| 2:B:303:LYS:HE2   | 2:B:303:LYS:H     | 1.83                     | 0.43              |
| 2:B:312:LEU:HG    | 2:B:316:THR:HG21  | 2.01                     | 0.43              |
| 3:C:29:PHE:HB2    | 3:C:32:ASN:HD21   | 1.82                     | 0.43              |
| 3:C:49:PHE:CZ     | 3:C:65:MET:HE3    | 2.53                     | 0.43              |
| 3:C:239:ILE:HD12  | 3:C:239:ILE:N     | 2.26                     | 0.43              |
| 7:G:115:GLN:HG3   | 7:G:116:GLN:HG3   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:206:GLU:OE1   | 1:A:206:GLU:N    | 2.46                     | 0.43              |
| 1:A:991:ASP:OD1   | 1:A:991:ASP:N    | 2.51                     | 0.43              |
| 3:C:337:LEU:HD12  | 11:K:104:MET:HE1 | 1.99                     | 0.43              |
| 4:D:39:GLN:CG     | 7:G:32:LYS:HE2   | 2.48                     | 0.43              |
| 4:D:57:PRO:C      | 4:D:59:ARG:H     | 2.25                     | 0.43              |
| 4:D:59:ARG:HB3    | 4:D:59:ARG:HH21  | 1.83                     | 0.43              |
| 15:O:170:ASP:OD1  | 15:O:170:ASP:N   | 2.48                     | 0.43              |
| 15:O:399:LEU:HD12 | 15:O:404:MET:HB3 | 2.00                     | 0.43              |
| 1:A:397:ASN:O     | 1:A:398:LYS:HB3  | 2.18                     | 0.43              |
| 1:A:618:ARG:HE    | 1:A:618:ARG:HB2  | 1.57                     | 0.43              |
| 1:A:691:LEU:HD12  | 1:A:691:LEU:HA   | 1.86                     | 0.43              |
| 2:B:562:MET:HE2   | 13:M:250:MET:HE3 | 2.00                     | 0.43              |
| 2:B:1049:GLU:H    | 2:B:1049:GLU:HG2 | 1.61                     | 0.43              |
| 2:B:1062:MET:HA   | 2:B:1062:MET:CE  | 2.43                     | 0.43              |
| 4:D:114:GLU:N     | 4:D:114:GLU:OE2  | 2.51                     | 0.43              |
| 15:O:89:PRO:HG2   | 17:Q:54:GLU:HG2  | 2.00                     | 0.43              |
| 1:A:90:LEU:HD23   | 1:A:90:LEU:HA    | 1.78                     | 0.43              |
| 1:A:530:VAL:HG13  | 1:A:535:GLY:HA2  | 2.00                     | 0.43              |
| 1:A:753:LEU:HD12  | 1:A:753:LEU:HA   | 1.81                     | 0.43              |
| 2:B:62:ASN:C      | 2:B:62:ASN:HD22  | 2.27                     | 0.43              |
| 2:B:78:LEU:N      | 2:B:78:LEU:HD12  | 2.34                     | 0.43              |
| 4:D:11:LEU:HD13   | 7:G:4:LEU:HD22   | 2.01                     | 0.43              |
| 4:D:48:GLU:HB2    | 7:G:103:PHE:O    | 2.16                     | 0.43              |
| 4:D:87:LEU:N      | 4:D:87:LEU:HD23  | 2.32                     | 0.43              |
| 4:D:96:GLU:H      | 4:D:96:GLU:HG2   | 1.43                     | 0.43              |
| 11:K:38:HIS:ND1   | 11:K:38:HIS:N    | 2.67                     | 0.43              |
| 12:L:15:MET:HE3   | 12:L:15:MET:HA   | 2.00                     | 0.43              |
| 13:M:238:LEU:HB3  | 14:N:341:LEU:O   | 2.19                     | 0.43              |
| 15:O:159:ARG:NH1  | 17:Q:112:PRO:O   | 2.50                     | 0.43              |
| 1:A:211:LEU:HA    | 15:O:411:LYS:HZ1 | 1.83                     | 0.43              |
| 1:A:727:TYR:CE1   | 1:A:751:LEU:HD11 | 2.53                     | 0.43              |
| 2:B:37:LYS:HA     | 2:B:41:LYS:HG2   | 2.00                     | 0.43              |
| 2:B:39:LEU:HD23   | 2:B:39:LEU:HA    | 1.91                     | 0.43              |
| 2:B:60:LYS:HD3    | 2:B:60:LYS:HA    | 1.81                     | 0.43              |
| 2:B:251:ILE:O     | 2:B:255:ILE:HG12 | 2.19                     | 0.43              |
| 2:B:674:TYR:HB3   | 2:B:677:HIS:HD2  | 1.83                     | 0.43              |
| 3:C:234:ARG:O     | 3:C:234:ARG:HG3  | 2.19                     | 0.43              |
| 15:O:409:ILE:HD12 | 15:O:423:LEU:CD1 | 2.31                     | 0.43              |
| 1:A:51:LEU:HD21   | 1:A:67:ARG:HD3   | 2.00                     | 0.43              |
| 1:A:384:VAL:HG22  | 1:A:480:VAL:HG12 | 2.01                     | 0.43              |
| 1:A:797:ALA:O     | 1:A:837:SER:HB3  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:899:GLN:HG2  | 1:A:1292:ASP:OD2  | 2.18                     | 0.43              |
| 1:A:1048:MET:HE3 | 1:A:1067:VAL:HG22 | 2.00                     | 0.43              |
| 1:A:1104:ARG:O   | 1:A:1203:GLY:HA2  | 2.18                     | 0.43              |
| 2:B:234:ILE:HB   | 2:B:239:ILE:HD11  | 1.99                     | 0.43              |
| 2:B:404:LYS:HD3  | 2:B:404:LYS:HA    | 1.57                     | 0.43              |
| 2:B:509:GLY:N    | 2:B:510:PRO:HD2   | 2.33                     | 0.43              |
| 2:B:606:VAL:HG12 | 2:B:608:ASN:H     | 1.84                     | 0.43              |
| 2:B:1105:ARG:HB2 | 2:B:1105:ARG:CZ   | 2.48                     | 0.43              |
| 3:C:72:ILE:HD13  | 11:K:106:VAL:HG11 | 2.01                     | 0.43              |
| 4:D:81:ALA:HB1   | 7:G:80:PHE:CE2    | 2.54                     | 0.43              |
| 15:O:416:ALA:N   | 15:O:417:PRO:CD   | 2.81                     | 0.43              |
| 1:A:171:LEU:HD21 | 1:A:329:PRO:HG3   | 1.99                     | 0.43              |
| 1:A:1083:PRO:HA  | 1:A:1249:ASN:OD1  | 2.19                     | 0.43              |
| 1:A:1198:LYS:H   | 1:A:1198:LYS:HG2  | 1.59                     | 0.43              |
| 1:A:1235:VAL:O   | 1:A:1235:VAL:CG1  | 2.66                     | 0.43              |
| 2:B:118:GLU:O    | 2:B:118:GLU:HG2   | 2.16                     | 0.43              |
| 2:B:175:GLU:H    | 2:B:175:GLU:HG2   | 1.55                     | 0.43              |
| 2:B:307:GLU:OE1  | 2:B:307:GLU:HA    | 2.18                     | 0.43              |
| 3:C:49:PHE:CE1   | 3:C:65:MET:HE3    | 2.54                     | 0.43              |
| 3:C:141:ARG:C    | 3:C:141:ARG:HD2   | 2.43                     | 0.43              |
| 4:D:5:ASP:HB2    | 7:G:6:GLU:CG      | 2.49                     | 0.43              |
| 17:Q:34:PRO:HG2  | 17:Q:37:LEU:HD23  | 2.01                     | 0.43              |
| 1:A:112:CYS:HB3  | 1:A:159:CYS:SG    | 2.59                     | 0.43              |
| 3:C:235:LEU:N    | 3:C:235:LEU:HD12  | 2.34                     | 0.43              |
| 4:D:95:VAL:HA    | 4:D:98:GLN:HB2    | 2.01                     | 0.43              |
| 5:E:10:LEU:HD21  | 5:E:52:ARG:HG2    | 2.00                     | 0.43              |
| 7:G:57:ALA:HA    | 7:G:68:THR:HG22   | 2.01                     | 0.43              |
| 15:O:413:PRO:O   | 15:O:415:HIS:HD2  | 2.01                     | 0.43              |
| 1:A:155:ILE:HG22 | 1:A:156:CYS:H     | 1.84                     | 0.43              |
| 1:A:1317:MET:HG3 | 1:A:1344:SER:HB2  | 1.99                     | 0.43              |
| 2:B:30:LEU:HD22  | 2:B:663:THR:CG2   | 2.49                     | 0.43              |
| 3:C:79:ILE:HG23  | 3:C:83:GLU:HB2    | 2.01                     | 0.43              |
| 7:G:151:ARG:C    | 7:G:151:ARG:CD    | 2.85                     | 0.43              |
| 18:R:11:G:H2'    | 18:R:11:G:N3      | 2.33                     | 0.43              |
| 1:A:55:VAL:HG21  | 1:A:280:THR:HG23  | 2.00                     | 0.42              |
| 1:A:174:ILE:HG22 | 1:A:218:LEU:HB2   | 2.00                     | 0.42              |
| 1:A:183:LYS:N    | 1:A:183:LYS:CD    | 2.80                     | 0.42              |
| 1:A:864:LYS:NZ   | 1:A:1048:MET:HB2  | 2.29                     | 0.42              |
| 2:B:192:GLU:O    | 2:B:192:GLU:CG    | 2.67                     | 0.42              |
| 2:B:246:GLU:O    | 2:B:247:SER:HB3   | 2.18                     | 0.42              |
| 3:C:315:VAL:HG12 | 3:C:316:LEU:HD22  | 1.99                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:52:LEU:HD13   | 1:A:52:LEU:HA     | 1.76                     | 0.42              |
| 1:A:116:MET:HG3   | 1:A:150:CYS:HB3   | 2.02                     | 0.42              |
| 2:B:274:LYS:HE2   | 2:B:274:LYS:HB3   | 1.90                     | 0.42              |
| 2:B:518:LEU:HD11  | 2:B:558:THR:HG21  | 2.00                     | 0.42              |
| 3:C:184:LEU:HD12  | 3:C:184:LEU:O     | 2.19                     | 0.42              |
| 11:K:92:ALA:C     | 11:K:95:PRO:HD2   | 2.44                     | 0.42              |
| 16:P:222:GLU:HA   | 16:P:225:ILE:HG22 | 2.01                     | 0.42              |
| 1:A:151:ARG:HH11  | 1:A:151:ARG:CG    | 2.33                     | 0.42              |
| 1:A:257:VAL:HA    | 1:A:258:PRO:HD3   | 1.79                     | 0.42              |
| 1:A:591:PRO:HD3   | 8:H:90:TYR:HA     | 2.01                     | 0.42              |
| 2:B:88:GLU:CD     | 2:B:88:GLU:N      | 2.76                     | 0.42              |
| 2:B:128:ARG:HD3   | 2:B:403:VAL:HG21  | 2.01                     | 0.42              |
| 2:B:372:LEU:HD21  | 2:B:415:MET:HA    | 1.99                     | 0.42              |
| 2:B:1108:TYR:CD1  | 2:B:1108:TYR:O    | 2.72                     | 0.42              |
| 18:R:10:U:H3'     | 18:R:11:G:C8      | 2.50                     | 0.42              |
| 19:X:39:DG:H2'    | 19:X:40:DC:C6     | 2.55                     | 0.42              |
| 1:A:94:HIS:HD2    | 1:A:96:GLY:H      | 1.66                     | 0.42              |
| 1:A:194:LEU:HD11  | 1:A:214:ALA:CB    | 2.49                     | 0.42              |
| 1:A:224:LEU:HG    | 1:A:251:ILE:HG12  | 2.01                     | 0.42              |
| 1:A:590:LYS:O     | 1:A:591:PRO:C     | 2.60                     | 0.42              |
| 1:A:1074:ILE:HD12 | 1:A:1290:LEU:HD21 | 2.01                     | 0.42              |
| 1:A:1080:ILE:HD11 | 1:A:1249:ASN:OD1  | 2.20                     | 0.42              |
| 2:B:395:GLN:HE21  | 2:B:395:GLN:HB3   | 1.63                     | 0.42              |
| 2:B:1092:CYS:C    | 2:B:1094:TYR:H    | 2.27                     | 0.42              |
| 4:D:17:PHE:CE1    | 4:D:21:THR:CG2    | 3.03                     | 0.42              |
| 2:B:712:LEU:HD23  | 2:B:712:LEU:HA    | 1.76                     | 0.42              |
| 15:O:370:LEU:HD23 | 15:O:370:LEU:HA   | 1.93                     | 0.42              |
| 15:O:459:ARG:H    | 15:O:459:ARG:HD3  | 1.85                     | 0.42              |
| 17:Q:34:PRO:HG2   | 17:Q:37:LEU:CD2   | 2.49                     | 0.42              |
| 1:A:1065:LEU:HD12 | 1:A:1065:LEU:HA   | 1.77                     | 0.42              |
| 2:B:1115:GLN:OE1  | 2:B:1115:GLN:N    | 2.53                     | 0.42              |
| 3:C:156:SER:HB2   | 3:C:162:LEU:HG    | 2.02                     | 0.42              |
| 3:C:235:LEU:HD23  | 3:C:303:ARG:HA    | 2.01                     | 0.42              |
| 4:D:69:PHE:HD1    | 4:D:69:PHE:O      | 2.02                     | 0.42              |
| 4:D:102:GLU:CD    | 4:D:102:GLU:H     | 2.25                     | 0.42              |
| 14:N:350:MET:HE3  | 14:N:350:MET:HB3  | 1.93                     | 0.42              |
| 15:O:124:LYS:HA   | 15:O:124:LYS:HD3  | 1.75                     | 0.42              |
| 16:P:220:ILE:O    | 16:P:224:GLY:N    | 2.50                     | 0.42              |
| 1:A:222:VAL:CG2   | 15:O:406:LEU:HD13 | 2.50                     | 0.42              |
| 1:A:553:THR:O     | 1:A:598:LYS:HE2   | 2.19                     | 0.42              |
| 1:A:735:LYS:HB2   | 1:A:735:LYS:HE2   | 1.90                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1185:MET:HB2  | 1:A:1186:TYR:H    | 1.63                     | 0.42              |
| 1:A:1372:PRO:HA   | 1:A:1373:PRO:HD3  | 1.89                     | 0.42              |
| 2:B:262:MET:HE3   | 2:B:262:MET:HB2   | 1.81                     | 0.42              |
| 4:D:2:GLU:HG2     | 4:D:2:GLU:O       | 2.19                     | 0.42              |
| 4:D:17:PHE:CD2    | 4:D:18:GLN:NE2    | 2.86                     | 0.42              |
| 6:F:81:VAL:HG11   | 6:F:96:GLU:HA     | 2.01                     | 0.42              |
| 7:G:197:LEU:HD13  | 7:G:200:TRP:CH2   | 2.54                     | 0.42              |
| 11:K:59:ILE:HG12  | 11:K:59:ILE:O     | 2.20                     | 0.42              |
| 15:O:459:ARG:NH1  | 15:O:460:LEU:HB2  | 2.34                     | 0.42              |
| 1:A:6:PHE:CD2     | 7:G:157:PHE:HA    | 2.54                     | 0.42              |
| 1:A:38:SER:HA     | 17:Q:24:GLY:HA2   | 2.02                     | 0.42              |
| 1:A:375:LEU:HD11  | 1:A:381:ALA:HB2   | 2.02                     | 0.42              |
| 1:A:533:ARG:O     | 1:A:1283:ASP:HB2  | 2.20                     | 0.42              |
| 2:B:28:ARG:HD3    | 2:B:28:ARG:HA     | 1.86                     | 0.42              |
| 4:D:3:VAL:O       | 4:D:3:VAL:CG2     | 2.68                     | 0.42              |
| 6:F:83:LEU:N      | 6:F:83:LEU:CD2    | 2.83                     | 0.42              |
| 12:L:26:ASN:ND2   | 12:L:36:CYS:HB3   | 2.35                     | 0.42              |
| 15:O:174:PRO:N    | 15:O:175:PRO:HD2  | 2.34                     | 0.42              |
| 1:A:942:LYS:HD2   | 1:A:942:LYS:HA    | 1.75                     | 0.42              |
| 1:A:1212:ILE:HD11 | 1:A:1223:TYR:CD2  | 2.53                     | 0.42              |
| 1:A:1343:VAL:HG21 | 2:B:1056:ILE:HD13 | 2.02                     | 0.42              |
| 2:B:253:GLN:CG    | 14:N:146:GLU:OE2  | 2.68                     | 0.42              |
| 4:D:48:GLU:CG     | 7:G:103:PHE:HB3   | 2.50                     | 0.42              |
| 4:D:65:ILE:C      | 4:D:65:ILE:HD12   | 2.44                     | 0.42              |
| 4:D:90:ARG:O      | 4:D:91:PRO:C      | 2.63                     | 0.42              |
| 7:G:38:VAL:HG11   | 7:G:186:LEU:HB2   | 2.02                     | 0.42              |
| 10:J:53:VAL:O     | 10:J:53:VAL:CG1   | 2.67                     | 0.42              |
| 15:O:170:ASP:CG   | 15:O:173:PRO:HG2  | 2.45                     | 0.42              |
| 19:X:39:DG:C2'    | 19:X:40:DC:H5'    | 2.42                     | 0.42              |
| 1:A:233:GLU:O     | 1:A:236:PRO:HD2   | 2.20                     | 0.42              |
| 1:A:324:GLU:OE2   | 1:A:343:GLN:NE2   | 2.53                     | 0.42              |
| 1:A:523:MET:HB3   | 1:A:523:MET:HE3   | 1.57                     | 0.42              |
| 1:A:700:ILE:O     | 1:A:704:THR:HG23  | 2.20                     | 0.42              |
| 2:B:131:LEU:HD22  | 2:B:131:LEU:HA    | 1.69                     | 0.42              |
| 15:O:409:ILE:HB   | 15:O:423:LEU:CG   | 2.49                     | 0.42              |
| 1:A:38:SER:CA     | 17:Q:24:GLY:HA2   | 2.50                     | 0.41              |
| 1:A:112:CYS:SG    | 1:A:159:CYS:SG    | 3.18                     | 0.41              |
| 1:A:1223:TYR:CD1  | 1:A:1223:TYR:N    | 2.88                     | 0.41              |
| 2:B:260:HIS:H     | 2:B:260:HIS:CD2   | 2.37                     | 0.41              |
| 2:B:494:LYS:HB2   | 2:B:494:LYS:HE2   | 1.67                     | 0.41              |
| 2:B:1062:MET:SD   | 7:G:61:PRO:HB3    | 2.60                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:89:VAL:O      | 5:E:92:GLN:HG3    | 2.19                     | 0.41              |
| 7:G:79:PRO:HG3    | 7:G:150:PHE:CE2   | 2.55                     | 0.41              |
| 13:M:207:HIS:O    | 14:N:370:THR:HA   | 2.20                     | 0.41              |
| 16:P:200:GLN:NE2  | 16:P:257:GLU:OE2  | 2.53                     | 0.41              |
| 16:P:206:ARG:CZ   | 16:P:217:TRP:HE1  | 2.33                     | 0.41              |
| 1:A:412:PRO:HG3   | 1:A:433:LYS:HB2   | 2.02                     | 0.41              |
| 1:A:1000:LEU:HD13 | 1:A:1000:LEU:HA   | 1.77                     | 0.41              |
| 2:B:640:ASP:OD1   | 2:B:640:ASP:N     | 2.53                     | 0.41              |
| 2:B:721:LYS:NZ    | 2:B:731:GLU:OE1   | 2.49                     | 0.41              |
| 2:B:1093:HIS:O    | 2:B:1093:HIS:CG   | 2.74                     | 0.41              |
| 4:D:28:LYS:HE2    | 4:D:28:LYS:HB3    | 1.83                     | 0.41              |
| 4:D:45:ILE:HG13   | 7:G:46:ILE:HG23   | 2.02                     | 0.41              |
| 4:D:66:VAL:O      | 4:D:70:LEU:HB2    | 2.20                     | 0.41              |
| 10:J:44:CYS:O     | 10:J:47:ARG:HG2   | 2.20                     | 0.41              |
| 15:O:102:THR:HA   | 15:O:129:LEU:HD11 | 2.02                     | 0.41              |
| 15:O:353:VAL:HG21 | 15:O:435:LEU:HD21 | 2.03                     | 0.41              |
| 15:O:399:LEU:CD1  | 15:O:404:MET:HB3  | 2.50                     | 0.41              |
| 1:A:662:ASN:O     | 1:A:666:ILE:HG12  | 2.20                     | 0.41              |
| 1:A:704:THR:HG22  | 1:A:839:TYR:CE1   | 2.56                     | 0.41              |
| 2:B:344:LEU:HD13  | 2:B:344:LEU:HA    | 1.80                     | 0.41              |
| 4:D:74:LYS:HB3    | 4:D:74:LYS:HE3    | 1.63                     | 0.41              |
| 13:M:123:GLU:HG3  | 13:M:125:HIS:CE1  | 2.55                     | 0.41              |
| 19:X:35:DT:H2'    | 19:X:36:DA:C8     | 2.55                     | 0.41              |
| 1:A:1050:LEU:HD23 | 1:A:1050:LEU:O    | 2.21                     | 0.41              |
| 1:A:1193:LYS:NZ   | 9:I:42:LYS:HD3    | 2.35                     | 0.41              |
| 2:B:241:LYS:HD3   | 2:B:246:GLU:HG2   | 2.01                     | 0.41              |
| 2:B:916:MET:HG3   | 2:B:917:PRO:HD2   | 2.02                     | 0.41              |
| 5:E:51:GLY:O      | 5:E:55:ARG:HB2    | 2.20                     | 0.41              |
| 1:A:232:ALA:HB2   | 15:O:6:ILE:HD11   | 2.03                     | 0.41              |
| 1:A:563:LYS:HE3   | 1:A:567:ILE:HD11  | 2.03                     | 0.41              |
| 1:A:625:CYS:SG    | 1:A:627:LYS:O     | 2.78                     | 0.41              |
| 2:B:236:ILE:HD12  | 2:B:240:PHE:HE2   | 1.86                     | 0.41              |
| 2:B:522:ASP:OD1   | 2:B:523:VAL:N     | 2.53                     | 0.41              |
| 2:B:551:ASP:OD1   | 2:B:551:ASP:N     | 2.50                     | 0.41              |
| 2:B:988:TYR:CD1   | 2:B:988:TYR:C     | 2.99                     | 0.41              |
| 11:K:27:LEU:HD23  | 11:K:27:LEU:N     | 2.36                     | 0.41              |
| 15:O:269:THR:HG21 | 15:O:298:PRO:HD3  | 2.01                     | 0.41              |
| 15:O:432:ALA:HB1  | 15:O:523:LEU:HD21 | 2.01                     | 0.41              |
| 16:P:227:LYS:HD2  | 16:P:240:ASN:HB3  | 2.03                     | 0.41              |
| 16:P:286:PRO:CB   | 17:Q:38:PHE:CD2   | 3.04                     | 0.41              |
| 1:A:94:HIS:HE1    | 2:B:1120:MET:O    | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:554:LEU:HD12  | 1:A:554:LEU:HA    | 1.77                     | 0.41              |
| 1:A:687:ALA:HB3   | 1:A:688:PRO:HD3   | 2.02                     | 0.41              |
| 1:A:864:LYS:NZ    | 1:A:1048:MET:CB   | 2.83                     | 0.41              |
| 2:B:513:LYS:HE3   | 2:B:513:LYS:HB2   | 1.72                     | 0.41              |
| 2:B:876:GLU:H     | 2:B:876:GLU:CD    | 2.24                     | 0.41              |
| 3:C:264:VAL:O     | 3:C:264:VAL:CG2   | 2.69                     | 0.41              |
| 6:F:100:ARG:NH2   | 6:F:123:LEU:O     | 2.54                     | 0.41              |
| 1:A:255:LEU:HD21  | 1:A:320:TYR:CE2   | 2.55                     | 0.41              |
| 1:A:717:LEU:HA    | 1:A:717:LEU:HD13  | 1.81                     | 0.41              |
| 2:B:133:ILE:HD13  | 2:B:380:PHE:CE2   | 2.56                     | 0.41              |
| 2:B:249:GLN:HE22  | 14:N:144:LYS:NZ   | 2.19                     | 0.41              |
| 4:D:48:GLU:CD     | 7:G:103:PHE:CD1   | 2.99                     | 0.41              |
| 4:D:94:ALA:HA     | 4:D:117:LEU:HD22  | 2.03                     | 0.41              |
| 13:M:239:VAL:HG13 | 14:N:343:LYS:NZ   | 2.35                     | 0.41              |
| 15:O:449:ARG:HB2  | 16:P:310:MET:HE1  | 2.01                     | 0.41              |
| 1:A:95:VAL:HG21   | 1:A:325:LEU:HD13  | 2.02                     | 0.41              |
| 1:A:1236:MET:HG3  | 5:E:137:ILE:HG21  | 2.02                     | 0.41              |
| 2:B:265:PHE:O     | 2:B:269:LEU:HG    | 2.21                     | 0.41              |
| 2:B:499:MET:HE2   | 2:B:663:THR:HG21  | 2.01                     | 0.41              |
| 3:C:287:ILE:CD1   | 3:C:293:LEU:CB    | 2.86                     | 0.41              |
| 15:O:376:GLU:HB3  | 15:O:424:TYR:HD1  | 1.86                     | 0.41              |
| 15:O:377:GLN:HA   | 15:O:380:VAL:HG12 | 2.03                     | 0.41              |
| 1:A:6:PHE:HZ      | 7:G:155:GLU:HB3   | 1.86                     | 0.41              |
| 1:A:259:PRO:O     | 1:A:262:ILE:HG12  | 2.20                     | 0.41              |
| 1:A:378:ASP:OD2   | 1:A:526:LYS:HE3   | 2.19                     | 0.41              |
| 1:A:1155:THR:O    | 1:A:1155:THR:CG2  | 2.68                     | 0.41              |
| 2:B:239:ILE:HG22  | 2:B:243:MET:HE2   | 2.02                     | 0.41              |
| 2:B:555:LEU:HD23  | 2:B:555:LEU:O     | 2.21                     | 0.41              |
| 2:B:686:GLN:HA    | 2:B:686:GLN:HE21  | 1.85                     | 0.41              |
| 2:B:957:ARG:HB2   | 2:B:957:ARG:HH11  | 1.86                     | 0.41              |
| 6:F:75:MET:HB2    | 7:G:15:PRO:HG2    | 2.01                     | 0.41              |
| 12:L:31:ARG:NE    | 12:L:31:ARG:HA    | 2.35                     | 0.41              |
| 1:A:6:PHE:CZ      | 7:G:155:GLU:HB3   | 2.56                     | 0.41              |
| 1:A:580:LYS:HB2   | 11:K:31:GLN:HG2   | 2.03                     | 0.41              |
| 1:A:1375:ARG:HA   | 1:A:1376:PRO:HD3  | 1.95                     | 0.41              |
| 2:B:618:TYR:HD1   | 2:B:618:TYR:HA    | 1.83                     | 0.41              |
| 4:D:54:SER:O      | 4:D:55:LYS:C      | 2.63                     | 0.41              |
| 4:D:100:MET:SD    | 7:G:147:GLU:CD    | 3.04                     | 0.41              |
| 11:K:28:GLU:OE1   | 11:K:28:GLU:N     | 2.54                     | 0.41              |
| 1:A:116:MET:O     | 1:A:153:LYS:HD3   | 2.21                     | 0.40              |
| 1:A:1121:PHE:HB2  | 9:I:38:VAL:HG13   | 2.02                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:548:VAL:O     | 2:B:548:VAL:HG12  | 2.20                     | 0.40              |
| 2:B:990:THR:HA    | 2:B:997:PRO:HA    | 2.03                     | 0.40              |
| 5:E:17:ILE:HD13   | 5:E:17:ILE:HA     | 1.89                     | 0.40              |
| 10:J:47:ARG:HH11  | 10:J:47:ARG:HG3   | 1.85                     | 0.40              |
| 11:K:50:THR:OG1   | 11:K:51:LEU:N     | 2.54                     | 0.40              |
| 11:K:106:VAL:O    | 11:K:110:VAL:HG12 | 2.21                     | 0.40              |
| 13:M:67:PRO:HD2   | 14:N:138:ILE:CG1  | 2.51                     | 0.40              |
| 1:A:39:LYS:HE3    | 1:A:41:LEU:HB2    | 2.03                     | 0.40              |
| 1:A:183:LYS:HD3   | 1:A:183:LYS:H     | 1.85                     | 0.40              |
| 1:A:963:ASP:N     | 1:A:963:ASP:OD1   | 2.54                     | 0.40              |
| 1:A:1304:THR:OG1  | 1:A:1306:PHE:N    | 2.51                     | 0.40              |
| 2:B:88:GLU:N      | 2:B:88:GLU:OE2    | 2.54                     | 0.40              |
| 2:B:196:LYS:HD3   | 20:Y:9:DA:OP1     | 2.20                     | 0.40              |
| 2:B:973:CYS:SG    | 2:B:974:GLU:N     | 2.94                     | 0.40              |
| 2:B:1078:ASP:HB3  | 2:B:1101:VAL:CG1  | 2.51                     | 0.40              |
| 4:D:16:VAL:HG21   | 7:G:2:PHE:CD2     | 2.57                     | 0.40              |
| 7:G:80:PHE:CD2    | 7:G:82:ASP:HB2    | 2.56                     | 0.40              |
| 9:I:8:CYS:HB2     | 13:M:139:PHE:CE1  | 2.56                     | 0.40              |
| 1:A:222:VAL:HG21  | 15:O:406:LEU:HD13 | 2.02                     | 0.40              |
| 1:A:263:ARG:HD3   | 1:A:279:LEU:HD23  | 2.02                     | 0.40              |
| 1:A:1364:HIS:ND1  | 1:A:1366:ALA:HB2  | 2.37                     | 0.40              |
| 2:B:1063:LEU:HD12 | 2:B:1063:LEU:O    | 2.21                     | 0.40              |
| 3:C:334:ARG:O     | 3:C:334:ARG:HD3   | 2.21                     | 0.40              |
| 9:I:1:MET:SD      | 14:N:153:GLN:OE1  | 2.79                     | 0.40              |
| 14:N:269:LEU:HA   | 14:N:383:LEU:O    | 2.20                     | 0.40              |
| 15:O:345:LEU:HB3  | 15:O:522:LEU:HD21 | 2.03                     | 0.40              |
| 15:O:356:GLU:O    | 16:P:289:LEU:HD11 | 2.21                     | 0.40              |
| 1:A:39:LYS:N      | 17:Q:24:GLY:CA    | 2.84                     | 0.40              |
| 1:A:406:LYS:HE2   | 1:A:406:LYS:HB3   | 1.96                     | 0.40              |
| 1:A:556:ASP:OD1   | 8:H:22:PHE:HB3    | 2.21                     | 0.40              |
| 1:A:973:ILE:HD13  | 1:A:973:ILE:HA    | 1.90                     | 0.40              |
| 1:A:1051:LYS:HE3  | 1:A:1051:LYS:C    | 2.44                     | 0.40              |
| 1:A:1134:LEU:HD12 | 1:A:1134:LEU:HA   | 1.94                     | 0.40              |
| 3:C:163:TYR:CE1   | 3:C:204:PRO:HG3   | 2.56                     | 0.40              |
| 4:D:3:VAL:HG11    | 7:G:42:VAL:HG21   | 2.02                     | 0.40              |
| 7:G:192:GLU:OE2   | 7:G:197:LEU:HD11  | 2.21                     | 0.40              |
| 13:M:67:PRO:HD2   | 14:N:138:ILE:HD11 | 2.02                     | 0.40              |
| 15:O:392:LYS:HD2  | 15:O:395:LEU:HD12 | 2.03                     | 0.40              |
| 15:O:514:ILE:HD11 | 17:Q:54:GLU:HG3   | 2.03                     | 0.40              |
| 17:Q:76:GLU:O     | 17:Q:78:PRO:HD3   | 2.22                     | 0.40              |
| 19:X:37:DG:H2''   | 19:X:38:DA:O5'    | 2.22                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:39:LYS:NZ     | 1:A:39:LYS:HB3    | 2.36                     | 0.40              |
| 1:A:133:GLY:O     | 1:A:138:GLN:NE2   | 2.52                     | 0.40              |
| 1:A:331:ASN:C     | 1:A:331:ASN:HD22  | 2.24                     | 0.40              |
| 1:A:860:ASP:OD1   | 2:B:465:VAL:HG21  | 2.22                     | 0.40              |
| 1:A:1216:GLU:OE1  | 1:A:1216:GLU:HA   | 2.20                     | 0.40              |
| 1:A:1363:LEU:HB3  | 6:F:105:ILE:HB    | 2.04                     | 0.40              |
| 2:B:404:LYS:NZ    | 2:B:404:LYS:N     | 2.69                     | 0.40              |
| 2:B:812:ASP:OD1   | 2:B:813:GLY:N     | 2.54                     | 0.40              |
| 7:G:5:VAL:HG12    | 7:G:7:MET:HG3     | 2.03                     | 0.40              |
| 9:I:4:PHE:HE2     | 14:N:146:GLU:OE1  | 2.05                     | 0.40              |
| 13:M:242:PRO:O    | 14:N:392:LEU:HD22 | 2.22                     | 0.40              |
| 14:N:389:PHE:O    | 14:N:393:LEU:HB3  | 2.22                     | 0.40              |
| 15:O:68:HIS:CE1   | 15:O:70:ARG:HH21  | 2.39                     | 0.40              |
| 15:O:106:ILE:HD13 | 15:O:125:VAL:HG11 | 2.03                     | 0.40              |
| 15:O:376:GLU:O    | 15:O:421:PHE:HE1  | 2.04                     | 0.40              |
| 17:Q:80:GLU:HA    | 17:Q:86:ARG:HD2   | 2.03                     | 0.40              |
| 17:Q:86:ARG:HB2   | 17:Q:86:ARG:CZ    | 2.51                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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     | 1356/1390 (98%) | 1274 (94%) | 69 (5%)  | 13 (1%)  | 12          | 45  |
| 2   | B     | 1091/1133 (96%) | 1026 (94%) | 57 (5%)  | 8 (1%)   | 18          | 51  |
| 3   | C     | 341/346 (99%)   | 338 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 4   | D     | 120/148 (81%)   | 109 (91%)  | 10 (8%)  | 1 (1%)   | 16          | 49  |
| 5   | E     | 207/210 (99%)   | 200 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 6   | F     | 74/127 (58%)    | 72 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 7   | G     | 160/204 (78%)   | 137 (86%)  | 23 (14%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 8   | H     | 146/150 (97%)   | 141 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 9   | I     | 105/108 (97%)   | 98 (93%)   | 7 (7%)   | 0        | 100         | 100 |
| 10  | J     | 63/67 (94%)     | 63 (100%)  | 0        | 0        | 100         | 100 |
| 11  | K     | 101/133 (76%)   | 100 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 12  | L     | 44/58 (76%)     | 42 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 13  | M     | 198/708 (28%)   | 189 (96%)  | 8 (4%)   | 1 (0%)   | 24          | 57  |
| 14  | N     | 140/398 (35%)   | 140 (100%) | 0        | 0        | 100         | 100 |
| 15  | O     | 435/534 (82%)   | 416 (96%)  | 18 (4%)  | 1 (0%)   | 43          | 72  |
| 16  | P     | 128/316 (40%)   | 102 (80%)  | 25 (20%) | 1 (1%)   | 16          | 49  |
| 17  | Q     | 82/223 (37%)    | 72 (88%)   | 9 (11%)  | 1 (1%)   | 10          | 41  |
| All | All   | 4791/6253 (77%) | 4519 (94%) | 246 (5%) | 26 (0%)  | 26          | 57  |

All (26) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 58   | HIS  |
| 1   | A     | 177  | GLU  |
| 1   | A     | 1185 | MET  |
| 1   | A     | 1209 | ARG  |
| 2   | B     | 1096 | LYS  |
| 4   | D     | 8    | SER  |
| 15  | O     | 409  | ILE  |
| 16  | P     | 296  | CYS  |
| 1   | A     | 485  | THR  |
| 1   | A     | 628  | GLY  |
| 1   | A     | 774  | SER  |
| 1   | A     | 988  | GLY  |
| 2   | B     | 247  | SER  |
| 2   | B     | 301  | PRO  |
| 1   | A     | 942  | LYS  |
| 2   | B     | 130  | ALA  |
| 2   | B     | 1099 | CYS  |
| 13  | M     | 228  | PRO  |
| 2   | B     | 64   | LYS  |
| 2   | B     | 123  | SER  |
| 2   | B     | 322  | PRO  |
| 17  | Q     | 28   | PRO  |
| 1   | A     | 38   | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 590  | LYS  |
| 1   | A     | 1125 | ASP  |
| 1   | A     | 1178 | ARG  |

### 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 PDB entries followed by that with respect to all EM entries.

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     | 1182/1212 (98%) | 1009 (85%) | 173 (15%) | 3           | 18  |
| 2   | B     | 950/988 (96%)   | 818 (86%)  | 132 (14%) | 3           | 19  |
| 3   | C     | 299/302 (99%)   | 275 (92%)  | 24 (8%)   | 11          | 37  |
| 4   | D     | 114/136 (84%)   | 88 (77%)   | 26 (23%)  | 1           | 6   |
| 5   | E     | 191/192 (100%)  | 184 (96%)  | 7 (4%)    | 30          | 56  |
| 6   | F     | 66/111 (60%)    | 60 (91%)   | 6 (9%)    | 9           | 33  |
| 7   | G     | 149/181 (82%)   | 145 (97%)  | 4 (3%)    | 39          | 61  |
| 8   | H     | 129/131 (98%)   | 129 (100%) | 0         | 100         | 100 |
| 9   | I     | 92/93 (99%)     | 92 (100%)  | 0         | 100         | 100 |
| 10  | J     | 53/56 (95%)     | 44 (83%)   | 9 (17%)   | 2           | 13  |
| 11  | K     | 92/119 (77%)    | 85 (92%)   | 7 (8%)    | 12          | 39  |
| 12  | L     | 43/55 (78%)     | 38 (88%)   | 5 (12%)   | 5           | 25  |
| 13  | M     | 180/622 (29%)   | 177 (98%)  | 3 (2%)    | 53          | 69  |
| 14  | N     | 131/347 (38%)   | 128 (98%)  | 3 (2%)    | 44          | 64  |
| 15  | O     | 400/476 (84%)   | 393 (98%)  | 7 (2%)    | 51          | 68  |
| 16  | P     | 114/280 (41%)   | 111 (97%)  | 3 (3%)    | 40          | 62  |
| 17  | Q     | 81/195 (42%)    | 74 (91%)   | 7 (9%)    | 10          | 34  |
| All | All   | 4266/5496 (78%) | 3850 (90%) | 416 (10%) | 10          | 31  |

All (416) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | PHE  |
| 1   | A     | 10  | ASP  |
| 1   | A     | 15  | ILE  |
| 1   | A     | 23  | LYS  |
| 1   | A     | 34  | ILE  |
| 1   | A     | 39  | LYS  |
| 1   | A     | 40  | ASN  |
| 1   | A     | 51  | LEU  |
| 1   | A     | 52  | LEU  |
| 1   | A     | 55  | VAL  |
| 1   | A     | 62  | THR  |
| 1   | A     | 71  | THR  |
| 1   | A     | 72  | CYS  |
| 1   | A     | 86  | ILE  |
| 1   | A     | 117 | LEU  |
| 1   | A     | 119 | GLN  |
| 1   | A     | 120 | GLU  |
| 1   | A     | 124 | GLN  |
| 1   | A     | 126 | LEU  |
| 1   | A     | 134 | LEU  |
| 1   | A     | 136 | TYR  |
| 1   | A     | 151 | ARG  |
| 1   | A     | 159 | CYS  |
| 1   | A     | 165 | THR  |
| 1   | A     | 171 | LEU  |
| 1   | A     | 179 | TYR  |
| 1   | A     | 189 | ILE  |
| 1   | A     | 190 | VAL  |
| 1   | A     | 193 | PHE  |
| 1   | A     | 194 | LEU  |
| 1   | A     | 205 | LYS  |
| 1   | A     | 211 | LEU  |
| 1   | A     | 221 | LEU  |
| 1   | A     | 222 | VAL  |
| 1   | A     | 224 | LEU  |
| 1   | A     | 225 | ASN  |
| 1   | A     | 226 | LEU  |
| 1   | A     | 237 | LEU  |
| 1   | A     | 240 | MET  |
| 1   | A     | 248 | SER  |
| 1   | A     | 251 | ILE  |
| 1   | A     | 257 | VAL  |
| 1   | A     | 263 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 293 | ILE  |
| 1   | A     | 303 | THR  |
| 1   | A     | 304 | GLN  |
| 1   | A     | 306 | ILE  |
| 1   | A     | 316 | GLN  |
| 1   | A     | 319 | LEU  |
| 1   | A     | 322 | ASN  |
| 1   | A     | 328 | ILE  |
| 1   | A     | 338 | THR  |
| 1   | A     | 351 | ARG  |
| 1   | A     | 367 | THR  |
| 1   | A     | 370 | SER  |
| 1   | A     | 377 | ILE  |
| 1   | A     | 421 | ILE  |
| 1   | A     | 426 | THR  |
| 1   | A     | 429 | LYS  |
| 1   | A     | 432 | LEU  |
| 1   | A     | 433 | LYS  |
| 1   | A     | 448 | ASP  |
| 1   | A     | 454 | LEU  |
| 1   | A     | 462 | PHE  |
| 1   | A     | 479 | ARG  |
| 1   | A     | 484 | ARG  |
| 1   | A     | 485 | THR  |
| 1   | A     | 507 | LEU  |
| 1   | A     | 520 | LEU  |
| 1   | A     | 523 | MET  |
| 1   | A     | 530 | VAL  |
| 1   | A     | 534 | ASN  |
| 1   | A     | 538 | LEU  |
| 1   | A     | 542 | ILE  |
| 1   | A     | 544 | ASP  |
| 1   | A     | 554 | LEU  |
| 1   | A     | 555 | LYS  |
| 1   | A     | 571 | ILE  |
| 1   | A     | 573 | VAL  |
| 1   | A     | 577 | GLU  |
| 1   | A     | 579 | ILE  |
| 1   | A     | 581 | VAL  |
| 1   | A     | 583 | LEU  |
| 1   | A     | 593 | THR  |
| 1   | A     | 596 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 623  | GLN  |
| 1   | A     | 627  | LYS  |
| 1   | A     | 630  | ASP  |
| 1   | A     | 646  | MET  |
| 1   | A     | 649  | SER  |
| 1   | A     | 663  | ILE  |
| 1   | A     | 668  | LEU  |
| 1   | A     | 685  | ARG  |
| 1   | A     | 686  | LEU  |
| 1   | A     | 707  | GLN  |
| 1   | A     | 709  | LEU  |
| 1   | A     | 717  | LEU  |
| 1   | A     | 729  | GLU  |
| 1   | A     | 731  | LEU  |
| 1   | A     | 748  | LEU  |
| 1   | A     | 751  | LEU  |
| 1   | A     | 768  | LEU  |
| 1   | A     | 771  | LEU  |
| 1   | A     | 773  | LYS  |
| 1   | A     | 798  | CYS  |
| 1   | A     | 799  | VAL  |
| 1   | A     | 822  | GLU  |
| 1   | A     | 876  | VAL  |
| 1   | A     | 881  | ASP  |
| 1   | A     | 882  | LEU  |
| 1   | A     | 883  | CYS  |
| 1   | A     | 897  | ILE  |
| 1   | A     | 901  | ILE  |
| 1   | A     | 908  | ASP  |
| 1   | A     | 912  | MET  |
| 1   | A     | 913  | GLU  |
| 1   | A     | 944  | GLU  |
| 1   | A     | 946  | ILE  |
| 1   | A     | 954  | LYS  |
| 1   | A     | 966  | LEU  |
| 1   | A     | 968  | GLU  |
| 1   | A     | 970  | LYS  |
| 1   | A     | 974  | LYS  |
| 1   | A     | 989  | ILE  |
| 1   | A     | 991  | ASP  |
| 1   | A     | 1000 | LEU  |
| 1   | A     | 1011 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1027 | MET  |
| 1   | A     | 1033 | VAL  |
| 1   | A     | 1048 | MET  |
| 1   | A     | 1050 | LEU  |
| 1   | A     | 1051 | LYS  |
| 1   | A     | 1054 | HIS  |
| 1   | A     | 1055 | PHE  |
| 1   | A     | 1058 | VAL  |
| 1   | A     | 1061 | MET  |
| 1   | A     | 1065 | LEU  |
| 1   | A     | 1067 | VAL  |
| 1   | A     | 1074 | ILE  |
| 1   | A     | 1088 | GLN  |
| 1   | A     | 1092 | ASP  |
| 1   | A     | 1093 | ASP  |
| 1   | A     | 1094 | ASP  |
| 1   | A     | 1096 | ASP  |
| 1   | A     | 1099 | ARG  |
| 1   | A     | 1113 | ILE  |
| 1   | A     | 1119 | GLU  |
| 1   | A     | 1126 | CYS  |
| 1   | A     | 1128 | ILE  |
| 1   | A     | 1129 | LEU  |
| 1   | A     | 1132 | LEU  |
| 1   | A     | 1137 | ILE  |
| 1   | A     | 1155 | THR  |
| 1   | A     | 1157 | LYS  |
| 1   | A     | 1170 | GLU  |
| 1   | A     | 1173 | VAL  |
| 1   | A     | 1180 | ASN  |
| 1   | A     | 1188 | VAL  |
| 1   | A     | 1191 | PHE  |
| 1   | A     | 1198 | LYS  |
| 1   | A     | 1200 | VAL  |
| 1   | A     | 1211 | VAL  |
| 1   | A     | 1212 | ILE  |
| 1   | A     | 1215 | ASP  |
| 1   | A     | 1225 | LEU  |
| 1   | A     | 1227 | VAL  |
| 1   | A     | 1230 | ASP  |
| 1   | A     | 1233 | ARG  |
| 1   | A     | 1241 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1242 | LYS  |
| 1   | A     | 1244 | THR  |
| 1   | A     | 1246 | THR  |
| 1   | A     | 1363 | LEU  |
| 2   | B     | 24   | GLU  |
| 2   | B     | 34   | LEU  |
| 2   | B     | 41   | LYS  |
| 2   | B     | 42   | GLN  |
| 2   | B     | 54   | GLU  |
| 2   | B     | 55   | ILE  |
| 2   | B     | 59   | MET  |
| 2   | B     | 62   | ASN  |
| 2   | B     | 65   | VAL  |
| 2   | B     | 74   | TYR  |
| 2   | B     | 81   | TYR  |
| 2   | B     | 95   | ARG  |
| 2   | B     | 115  | VAL  |
| 2   | B     | 119  | TYR  |
| 2   | B     | 120  | THR  |
| 2   | B     | 121  | ARG  |
| 2   | B     | 125  | ARG  |
| 2   | B     | 131  | LEU  |
| 2   | B     | 138  | ILE  |
| 2   | B     | 139  | MET  |
| 2   | B     | 140  | LEU  |
| 2   | B     | 148  | THR  |
| 2   | B     | 181  | GLN  |
| 2   | B     | 183  | GLN  |
| 2   | B     | 189  | ILE  |
| 2   | B     | 191  | VAL  |
| 2   | B     | 203  | VAL  |
| 2   | B     | 204  | THR  |
| 2   | B     | 207  | THR  |
| 2   | B     | 213  | ARG  |
| 2   | B     | 214  | THR  |
| 2   | B     | 216  | MET  |
| 2   | B     | 218  | VAL  |
| 2   | B     | 232  | GLU  |
| 2   | B     | 233  | ASP  |
| 2   | B     | 234  | ILE  |
| 2   | B     | 238  | ILE  |
| 2   | B     | 254  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 271 | GLU  |
| 2   | B     | 279 | THR  |
| 2   | B     | 303 | LYS  |
| 2   | B     | 305 | LYS  |
| 2   | B     | 306 | ILE  |
| 2   | B     | 316 | THR  |
| 2   | B     | 317 | ILE  |
| 2   | B     | 319 | THR  |
| 2   | B     | 343 | ILE  |
| 2   | B     | 344 | LEU  |
| 2   | B     | 348 | ASP  |
| 2   | B     | 351 | VAL  |
| 2   | B     | 375 | ASP  |
| 2   | B     | 377 | PHE  |
| 2   | B     | 382 | SER  |
| 2   | B     | 384 | MET  |
| 2   | B     | 387 | ILE  |
| 2   | B     | 392 | ILE  |
| 2   | B     | 394 | LYS  |
| 2   | B     | 402 | VAL  |
| 2   | B     | 404 | LYS  |
| 2   | B     | 409 | ASP  |
| 2   | B     | 411 | ILE  |
| 2   | B     | 412 | THR  |
| 2   | B     | 419 | ILE  |
| 2   | B     | 440 | LEU  |
| 2   | B     | 446 | ILE  |
| 2   | B     | 462 | THR  |
| 2   | B     | 463 | ARG  |
| 2   | B     | 494 | LYS  |
| 2   | B     | 502 | ILE  |
| 2   | B     | 505 | ASP  |
| 2   | B     | 506 | MET  |
| 2   | B     | 507 | GLU  |
| 2   | B     | 517 | ASN  |
| 2   | B     | 518 | LEU  |
| 2   | B     | 525 | LEU  |
| 2   | B     | 530 | GLU  |
| 2   | B     | 536 | VAL  |
| 2   | B     | 542 | ASN  |
| 2   | B     | 548 | VAL  |
| 2   | B     | 549 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 552 | HIS  |
| 2   | B     | 559 | PHE  |
| 2   | B     | 561 | LEU  |
| 2   | B     | 570 | GLU  |
| 2   | B     | 573 | SER  |
| 2   | B     | 574 | ILE  |
| 2   | B     | 578 | LEU  |
| 2   | B     | 583 | VAL  |
| 2   | B     | 606 | VAL  |
| 2   | B     | 616 | GLN  |
| 2   | B     | 619 | ARG  |
| 2   | B     | 623 | ASP  |
| 2   | B     | 640 | ASP  |
| 2   | B     | 643 | ILE  |
| 2   | B     | 686 | GLN  |
| 2   | B     | 697 | ILE  |
| 2   | B     | 708 | LEU  |
| 2   | B     | 712 | LEU  |
| 2   | B     | 724 | THR  |
| 2   | B     | 733 | LEU  |
| 2   | B     | 743 | VAL  |
| 2   | B     | 764 | ARG  |
| 2   | B     | 771 | VAL  |
| 2   | B     | 777 | CYS  |
| 2   | B     | 784 | ASN  |
| 2   | B     | 790 | VAL  |
| 2   | B     | 791 | MET  |
| 2   | B     | 800 | ARG  |
| 2   | B     | 801 | LYS  |
| 2   | B     | 814 | ILE  |
| 2   | B     | 815 | CYS  |
| 2   | B     | 817 | PRO  |
| 2   | B     | 822 | GLU  |
| 2   | B     | 828 | VAL  |
| 2   | B     | 874 | ASN  |
| 2   | B     | 883 | MET  |
| 2   | B     | 885 | LEU  |
| 2   | B     | 906 | VAL  |
| 2   | B     | 916 | MET  |
| 2   | B     | 946 | LEU  |
| 2   | B     | 976 | LEU  |
| 2   | B     | 984 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 990  | THR  |
| 2   | B     | 1007 | VAL  |
| 2   | B     | 1010 | GLN  |
| 2   | B     | 1030 | VAL  |
| 2   | B     | 1049 | GLU  |
| 2   | B     | 1089 | SER  |
| 2   | B     | 1112 | LEU  |
| 2   | B     | 1113 | LEU  |
| 2   | B     | 1115 | GLN  |
| 2   | B     | 1128 | LEU  |
| 3   | C     | 21   | VAL  |
| 3   | C     | 26   | THR  |
| 3   | C     | 34   | SER  |
| 3   | C     | 43   | ASP  |
| 3   | C     | 52   | ASP  |
| 3   | C     | 54   | VAL  |
| 3   | C     | 55   | HIS  |
| 3   | C     | 90   | GLU  |
| 3   | C     | 95   | TYR  |
| 3   | C     | 100  | ILE  |
| 3   | C     | 103  | ASP  |
| 3   | C     | 126  | ASN  |
| 3   | C     | 147  | THR  |
| 3   | C     | 158  | ASP  |
| 3   | C     | 164  | VAL  |
| 3   | C     | 183  | ASP  |
| 3   | C     | 215  | VAL  |
| 3   | C     | 230  | THR  |
| 3   | C     | 261  | VAL  |
| 3   | C     | 270  | LYS  |
| 3   | C     | 272  | VAL  |
| 3   | C     | 316  | LEU  |
| 3   | C     | 319  | ASP  |
| 3   | C     | 320  | VAL  |
| 4   | D     | 1    | MET  |
| 4   | D     | 3    | VAL  |
| 4   | D     | 11   | LEU  |
| 4   | D     | 14   | TYR  |
| 4   | D     | 15   | GLU  |
| 4   | D     | 18   | GLN  |
| 4   | D     | 19   | LEU  |
| 4   | D     | 20   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 32  | LYS  |
| 4   | D     | 40  | GLN  |
| 4   | D     | 41  | ASN  |
| 4   | D     | 43  | ASN  |
| 4   | D     | 59  | ARG  |
| 4   | D     | 64  | GLU  |
| 4   | D     | 65  | ILE  |
| 4   | D     | 70  | LEU  |
| 4   | D     | 74  | LYS  |
| 4   | D     | 77  | LYS  |
| 4   | D     | 84  | LEU  |
| 4   | D     | 88  | ASN  |
| 4   | D     | 96  | GLU  |
| 4   | D     | 97  | ILE  |
| 4   | D     | 99  | LEU  |
| 4   | D     | 101 | VAL  |
| 4   | D     | 105 | GLU  |
| 4   | D     | 113 | ILE  |
| 5   | E     | 28  | VAL  |
| 5   | E     | 50  | GLU  |
| 5   | E     | 55  | ARG  |
| 5   | E     | 61  | LEU  |
| 5   | E     | 76  | PHE  |
| 5   | E     | 79  | GLU  |
| 5   | E     | 177 | ASP  |
| 6   | F     | 52  | ILE  |
| 6   | F     | 80  | MET  |
| 6   | F     | 81  | VAL  |
| 6   | F     | 82  | GLU  |
| 6   | F     | 107 | ARG  |
| 6   | F     | 116 | GLU  |
| 7   | G     | 22  | LEU  |
| 7   | G     | 59  | VAL  |
| 7   | G     | 152 | VAL  |
| 7   | G     | 198 | LEU  |
| 10  | J     | 3   | ILE  |
| 10  | J     | 5   | VAL  |
| 10  | J     | 9   | THR  |
| 10  | J     | 19  | GLU  |
| 10  | J     | 21  | TYR  |
| 10  | J     | 26  | GLN  |
| 10  | J     | 30  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | J     | 33  | ASP  |
| 10  | J     | 48  | MET  |
| 11  | K     | 27  | LEU  |
| 11  | K     | 38  | HIS  |
| 11  | K     | 71  | THR  |
| 11  | K     | 77  | GLU  |
| 11  | K     | 82  | LEU  |
| 11  | K     | 103 | LEU  |
| 11  | K     | 110 | VAL  |
| 12  | L     | 19  | CYS  |
| 12  | L     | 28  | ILE  |
| 12  | L     | 34  | ILE  |
| 12  | L     | 52  | LEU  |
| 12  | L     | 53  | VAL  |
| 13  | M     | 7   | ASP  |
| 13  | M     | 233 | VAL  |
| 13  | M     | 239 | VAL  |
| 14  | N     | 269 | LEU  |
| 14  | N     | 393 | LEU  |
| 14  | N     | 395 | HIS  |
| 15  | O     | 170 | ASP  |
| 15  | O     | 239 | LEU  |
| 15  | O     | 408 | GLU  |
| 15  | O     | 409 | ILE  |
| 15  | O     | 411 | LYS  |
| 15  | O     | 414 | ASP  |
| 15  | O     | 423 | LEU  |
| 16  | P     | 205 | GLN  |
| 16  | P     | 283 | VAL  |
| 16  | P     | 284 | ARG  |
| 17  | Q     | 27  | LEU  |
| 17  | Q     | 31  | VAL  |
| 17  | Q     | 79  | GLU  |
| 17  | Q     | 80  | GLU  |
| 17  | Q     | 83  | ASP  |
| 17  | Q     | 86  | ARG  |
| 17  | Q     | 87  | TYR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 17  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 30   | GLN  |
| 1   | A     | 58   | HIS  |
| 1   | A     | 94   | HIS  |
| 1   | A     | 138  | GLN  |
| 1   | A     | 157  | HIS  |
| 1   | A     | 163  | ASN  |
| 1   | A     | 203  | HIS  |
| 1   | A     | 225  | ASN  |
| 1   | A     | 241  | ASN  |
| 1   | A     | 296  | HIS  |
| 1   | A     | 314  | GLN  |
| 1   | A     | 316  | GLN  |
| 1   | A     | 322  | ASN  |
| 1   | A     | 331  | ASN  |
| 1   | A     | 349  | GLN  |
| 1   | A     | 423  | GLN  |
| 1   | A     | 442  | GLN  |
| 1   | A     | 453  | HIS  |
| 1   | A     | 463  | ASN  |
| 1   | A     | 511  | GLN  |
| 1   | A     | 534  | ASN  |
| 1   | A     | 543  | GLN  |
| 1   | A     | 611  | ASN  |
| 1   | A     | 623  | GLN  |
| 1   | A     | 673  | GLN  |
| 1   | A     | 707  | GLN  |
| 1   | A     | 762  | HIS  |
| 1   | A     | 791  | ASN  |
| 1   | A     | 794  | GLN  |
| 1   | A     | 824  | HIS  |
| 1   | A     | 836  | ASN  |
| 1   | A     | 872  | GLN  |
| 1   | A     | 899  | GLN  |
| 1   | A     | 1039 | GLN  |
| 1   | A     | 1047 | GLN  |
| 1   | A     | 1062 | ASN  |
| 1   | A     | 1180 | ASN  |
| 1   | A     | 1239 | HIS  |
| 1   | A     | 1277 | ASN  |
| 1   | A     | 1278 | HIS  |
| 1   | A     | 1327 | HIS  |
| 1   | A     | 1336 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 62   | ASN  |
| 2   | B     | 92   | ASN  |
| 2   | B     | 187  | ASN  |
| 2   | B     | 249  | GLN  |
| 2   | B     | 260  | HIS  |
| 2   | B     | 276  | GLN  |
| 2   | B     | 320  | HIS  |
| 2   | B     | 395  | GLN  |
| 2   | B     | 423  | ASN  |
| 2   | B     | 434  | GLN  |
| 2   | B     | 458  | GLN  |
| 2   | B     | 495  | ASN  |
| 2   | B     | 542  | ASN  |
| 2   | B     | 569  | ASN  |
| 2   | B     | 577  | ASN  |
| 2   | B     | 602  | GLN  |
| 2   | B     | 608  | ASN  |
| 2   | B     | 620  | ASN  |
| 2   | B     | 626  | HIS  |
| 2   | B     | 677  | HIS  |
| 2   | B     | 686  | GLN  |
| 2   | B     | 692  | GLN  |
| 2   | B     | 703  | ASN  |
| 2   | B     | 738  | ASN  |
| 2   | B     | 887  | GLN  |
| 2   | B     | 1093 | HIS  |
| 2   | B     | 1118 | GLN  |
| 3   | C     | 32   | ASN  |
| 3   | C     | 48   | ASN  |
| 3   | C     | 180  | ASN  |
| 4   | D     | 7    | ASN  |
| 4   | D     | 35   | HIS  |
| 4   | D     | 39   | GLN  |
| 4   | D     | 43   | ASN  |
| 4   | D     | 60   | HIS  |
| 4   | D     | 61   | GLN  |
| 4   | D     | 85   | GLN  |
| 4   | D     | 89   | HIS  |
| 4   | D     | 98   | GLN  |
| 8   | H     | 29   | HIS  |
| 8   | H     | 76   | ASN  |
| 8   | H     | 131  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | I     | 10  | ASN  |
| 9   | I     | 21  | HIS  |
| 9   | I     | 61  | ASN  |
| 10  | J     | 26  | GLN  |
| 11  | K     | 45  | HIS  |
| 12  | L     | 26  | ASN  |
| 13  | M     | 125 | HIS  |
| 14  | N     | 270 | GLN  |
| 15  | O     | 3   | GLN  |
| 15  | O     | 14  | GLN  |
| 15  | O     | 49  | GLN  |
| 15  | O     | 113 | ASN  |
| 15  | O     | 146 | ASN  |
| 15  | O     | 337 | ASN  |
| 15  | O     | 355 | GLN  |
| 15  | O     | 379 | GLN  |
| 15  | O     | 415 | HIS  |
| 15  | O     | 445 | ASN  |
| 15  | O     | 457 | ASN  |
| 15  | O     | 465 | GLN  |
| 15  | O     | 507 | ASN  |
| 16  | P     | 200 | GLN  |
| 16  | P     | 207 | ASN  |
| 16  | P     | 240 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed   | Backbone Outliers | Pucker Outliers |
|-----|-------|------------|-------------------|-----------------|
| 18  | R     | 4/10 (40%) | 3 (75%)           | 1 (25%)         |

All (3) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | R     | 9   | C    |
| 18  | R     | 10  | U    |
| 18  | R     | 11  | G    |

All (1) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | R     | 8   | G    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 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 | $\# Z  > 2$ |
| 23  | SF4  | P     | 401 | 16   | 0,12,12      | -    | -           | -           |      |             |

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   |
|-----|------|-------|-----|------|---------|----------|---------|
| 23  | SF4  | P     | 401 | 16   | -       | -        | 0/6/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

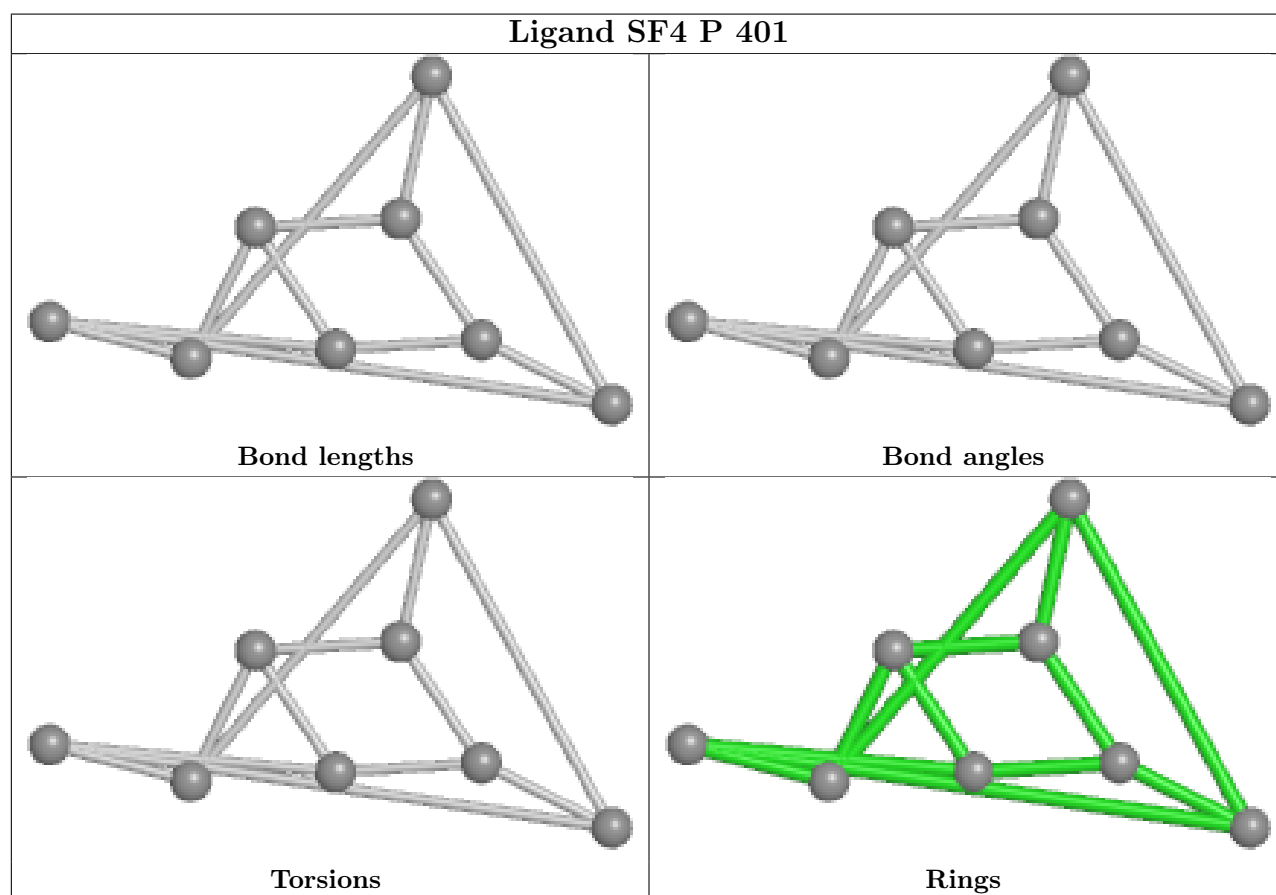
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23  | P     | 401 | SF4  | 4       | 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 [i](#)

There are no chain breaks in this entry.

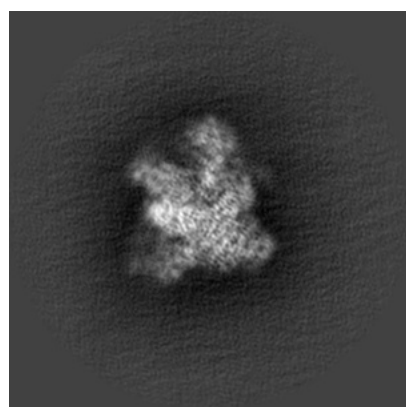
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31622. These allow visual inspection of the internal detail of the map and identification of artifacts.

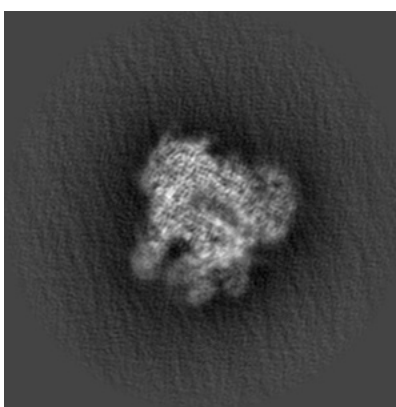
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

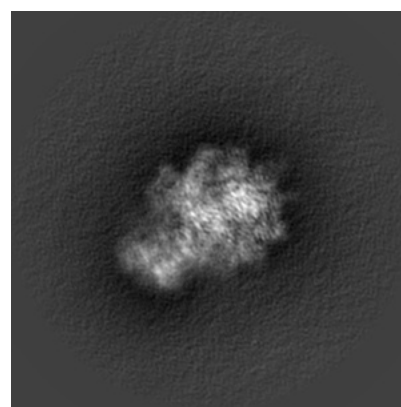
#### 6.1.1 Primary map



X



Y

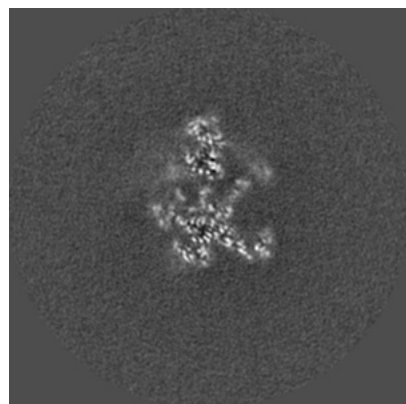


Z

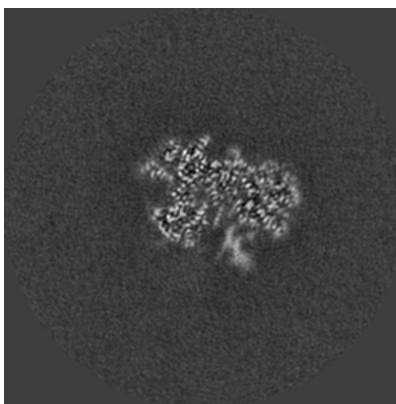
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

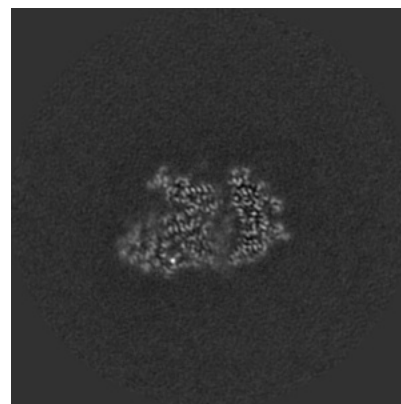
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

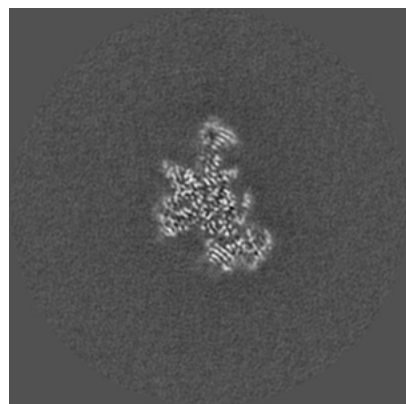


Z Index: 180

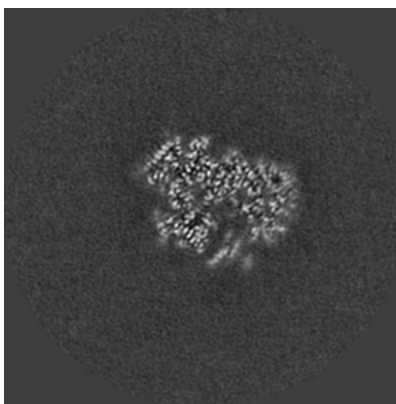
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

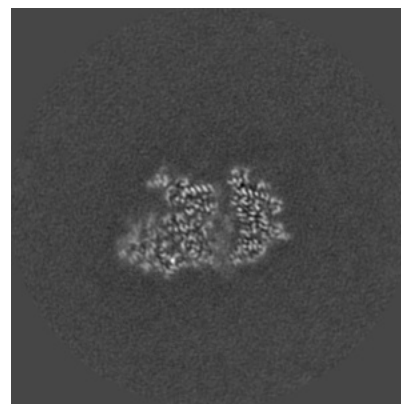
### 6.3.1 Primary map



X Index: 208



Y Index: 185

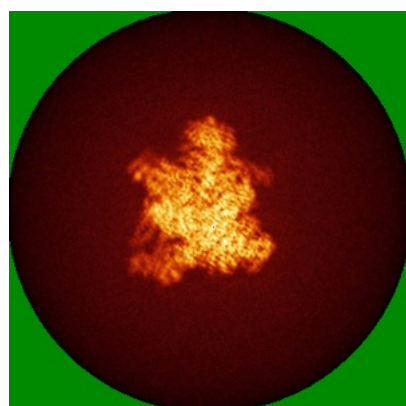


Z Index: 179

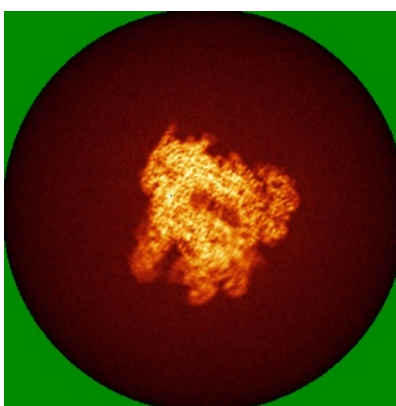
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

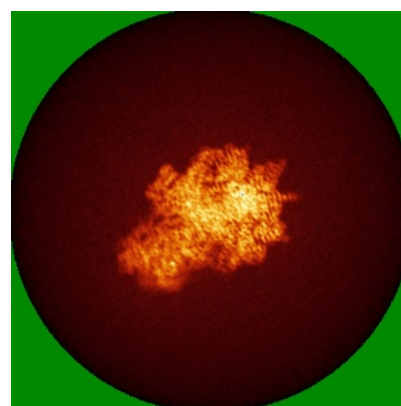
### 6.4.1 Primary map



X



Y

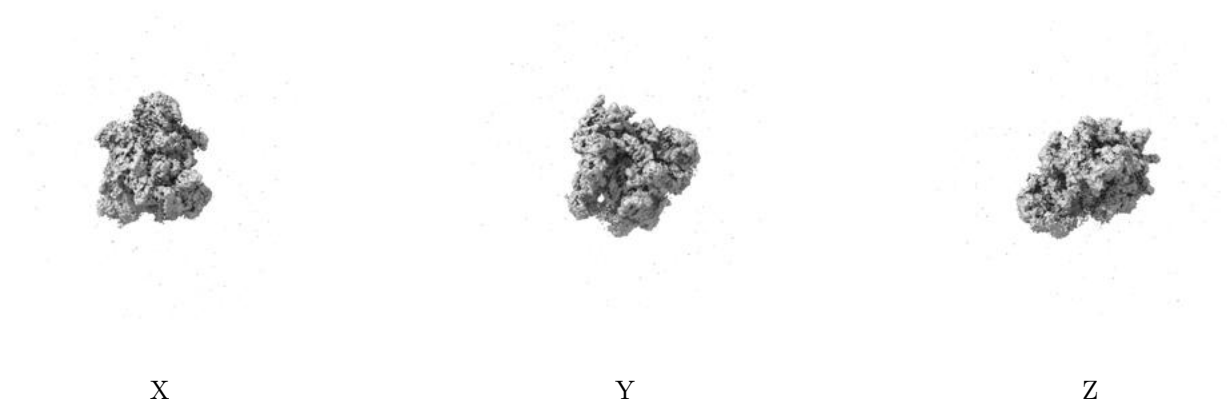


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

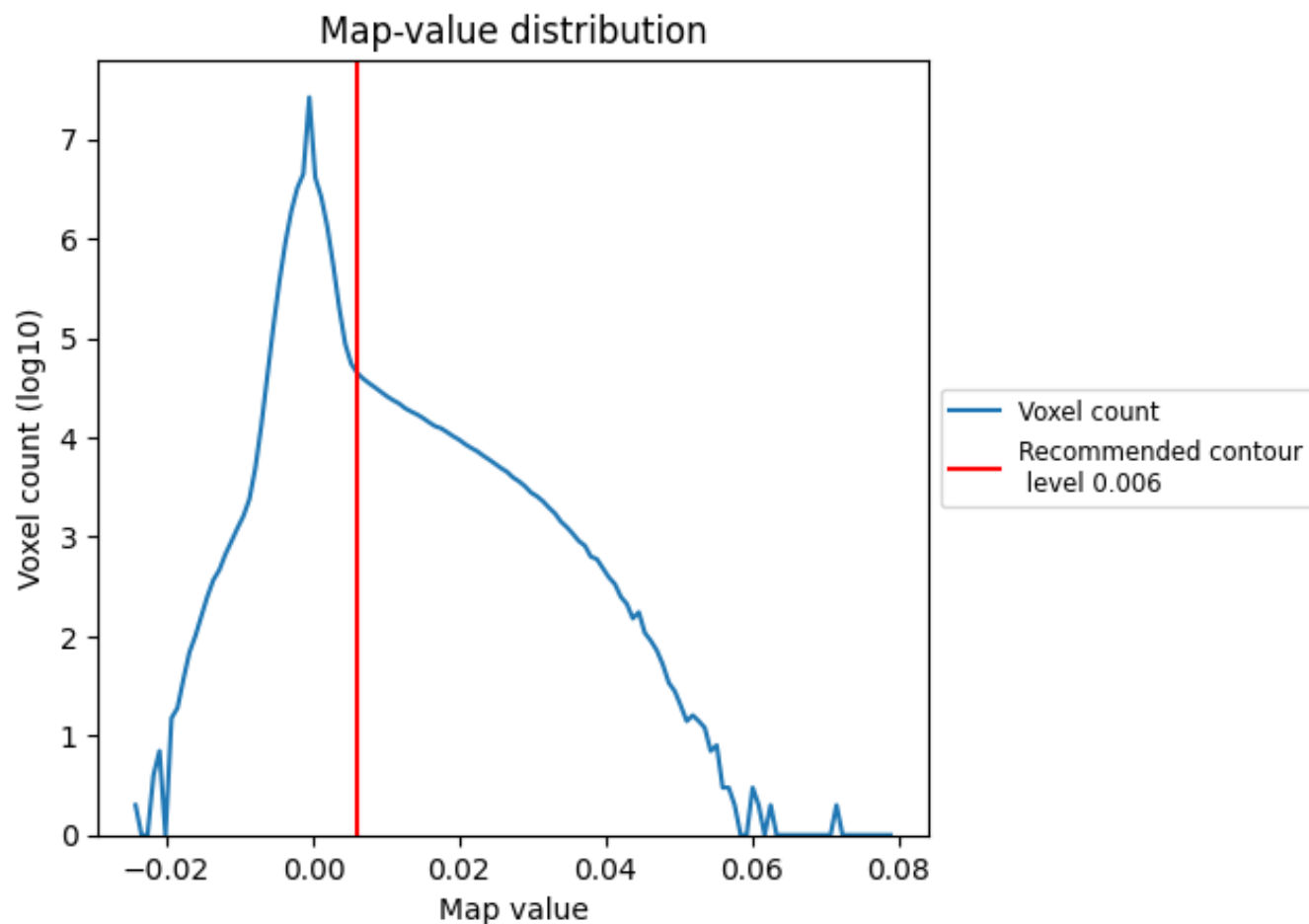
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

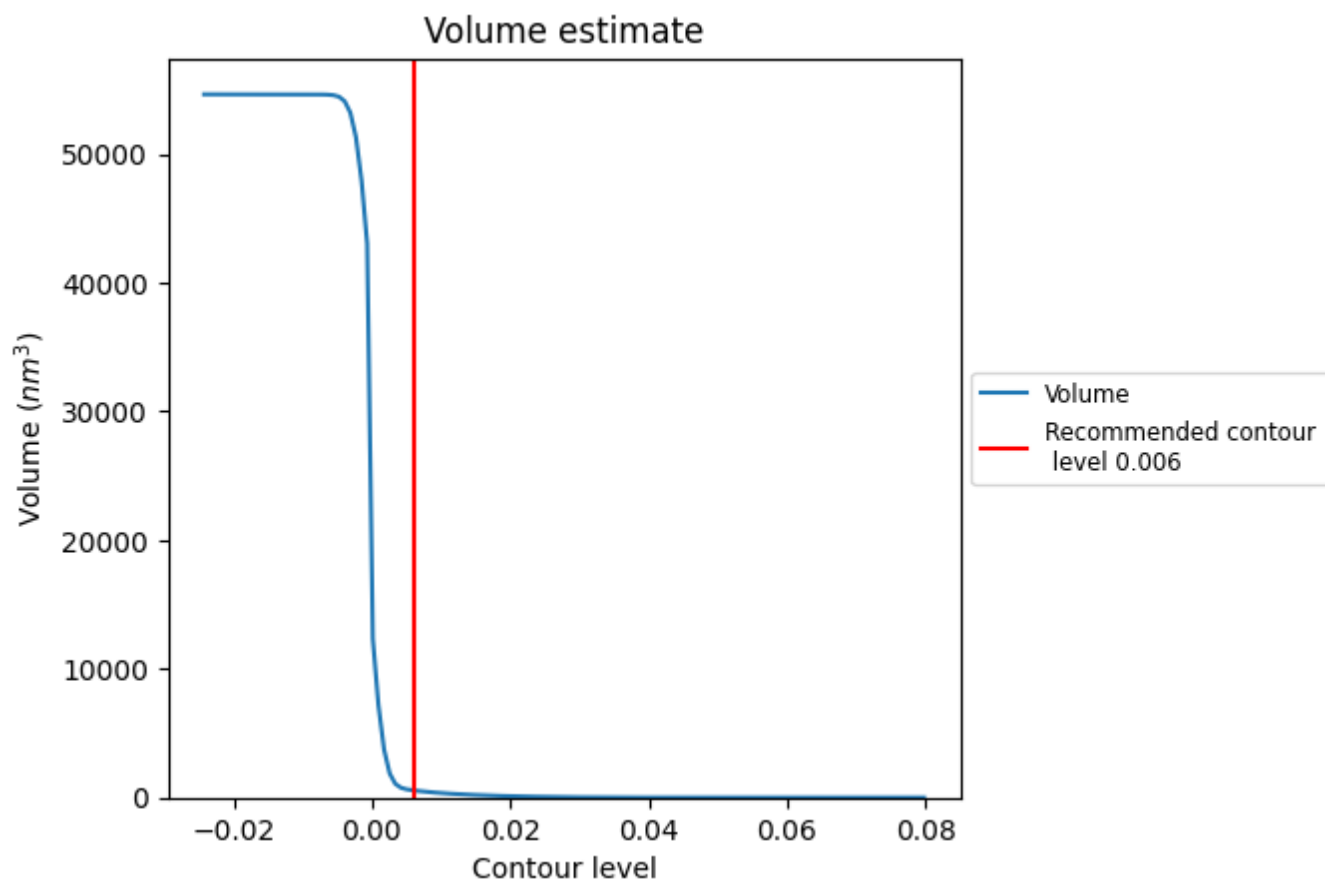
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

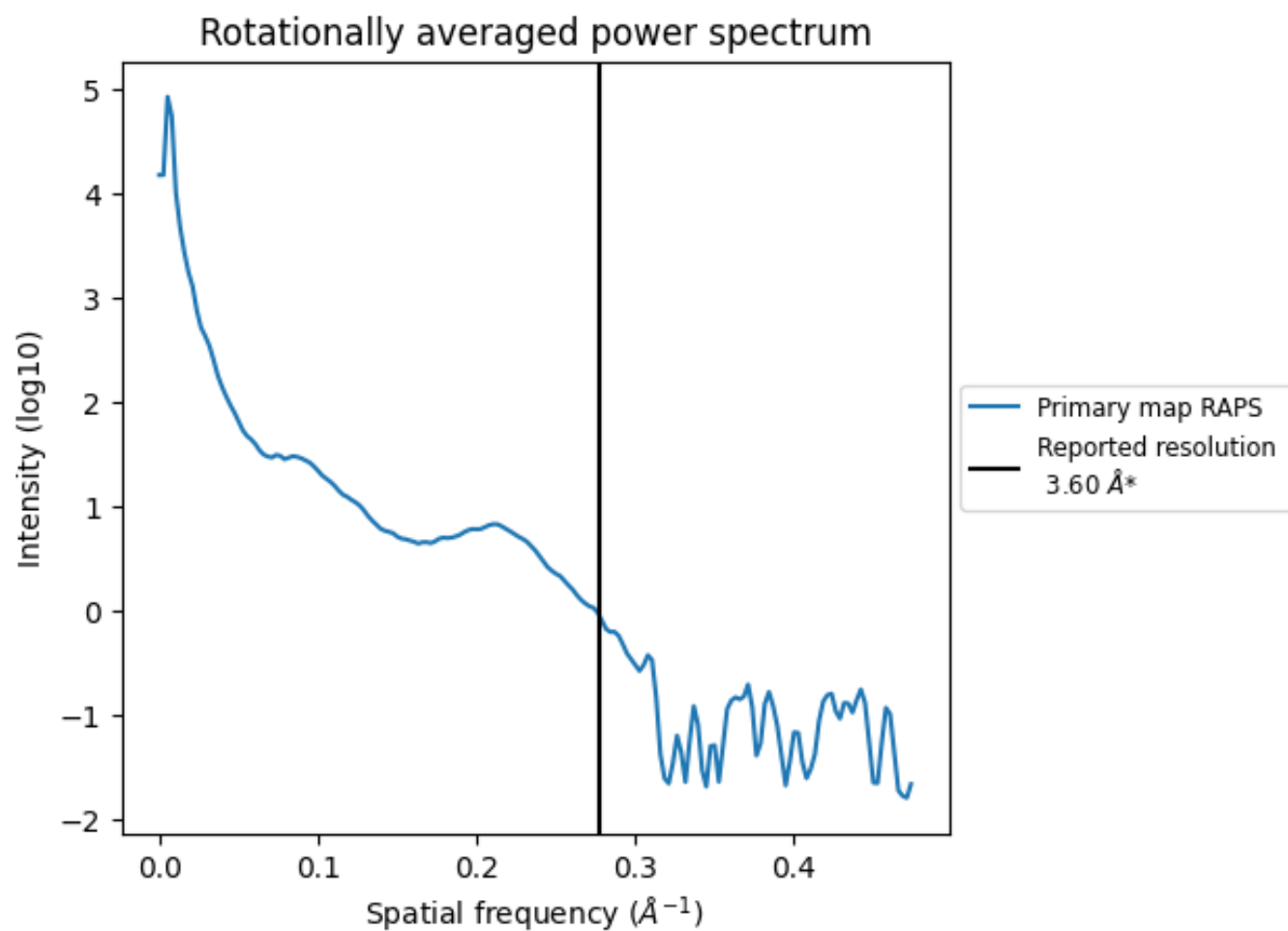
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 558  $\text{nm}^3$ ; this corresponds to an approximate mass of 504 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

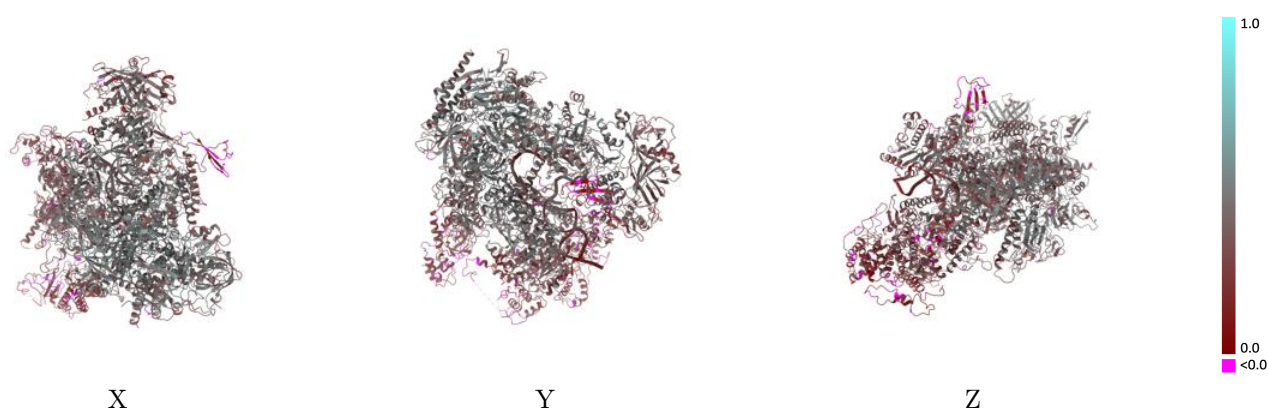
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31622 and PDB model 7FJJ. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlay [i](#)

This section was not generated.

### 9.2 Q-score mapped to coordinate model [i](#)

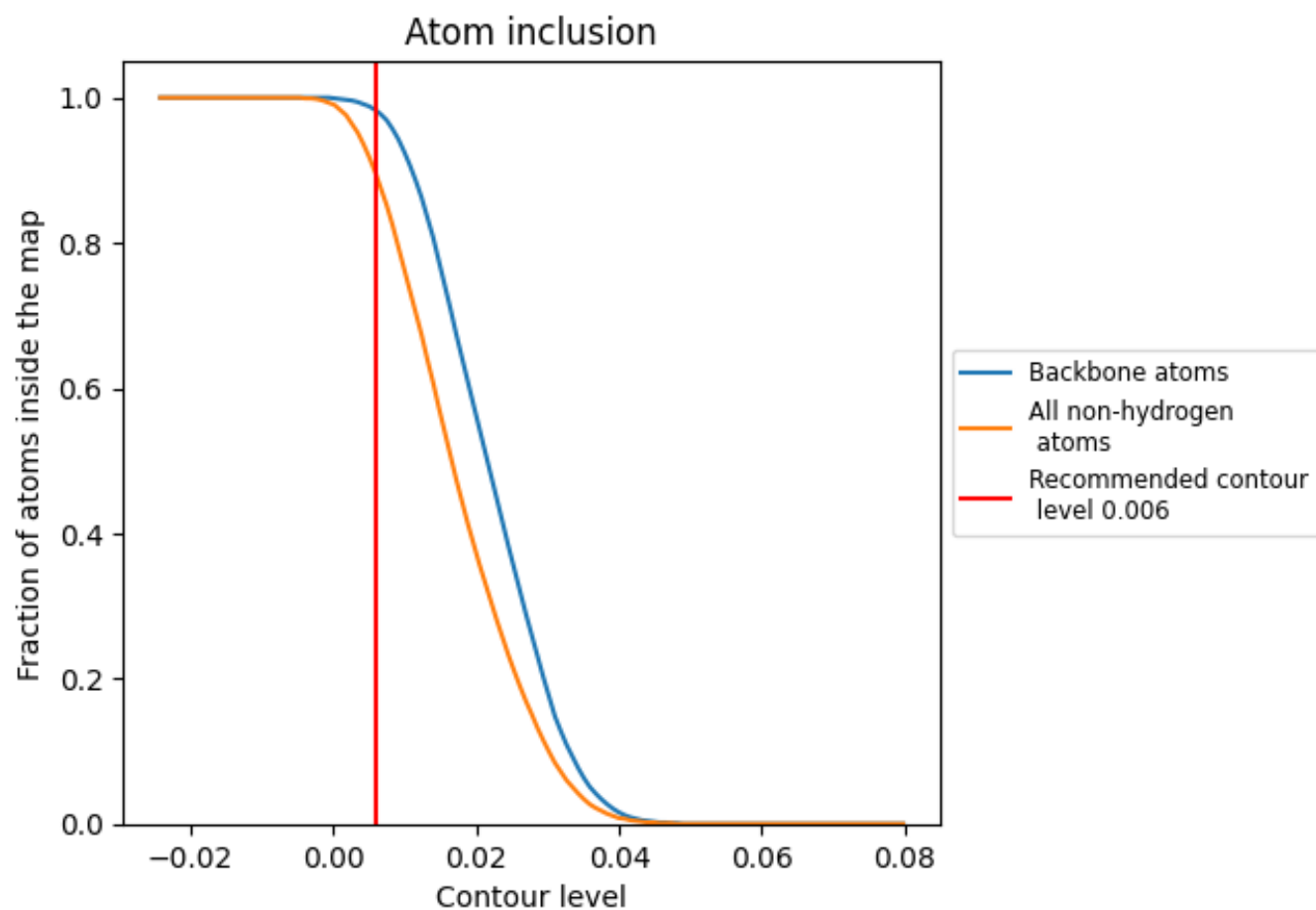


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

### 9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8930   |  0.3640   |
| A     |  0.9020   |  0.4020   |
| B     |  0.9170   |  0.4430   |
| C     |  0.9430   |  0.4410   |
| D     |  0.8260   |  0.1330   |
| E     |  0.9150   |  0.3810   |
| F     |  0.9320   |  0.4450   |
| G     |  0.8720   |  0.2100   |
| H     |  0.9210   |  0.4220   |
| I     |  0.7580   |  0.2130   |
| J     |  0.9440   |  0.4590   |
| K     |  0.9320   |  0.4180   |
| L     |  0.9250   |  0.3950   |
| M     |  0.8760   |  0.3480   |
| N     |  0.8350  |  0.3380  |
| O     |  0.8560 |  0.2120 |
| P     |  0.8440 |  0.1840 |
| Q     |  0.6810 |  0.1280 |
| R     |  0.4880 |  0.1650 |
| X     |  0.9380 |  0.3380 |
| Y     |  0.9530 |  0.2890 |

