



## Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 02:29 pm BST

PDB ID : 7ADD / pdb\_00007add  
EMDB ID : EMD-11724  
Title : Transcription termination intermediate complex IIIa  
Authors : Said, N.; Hilal, T.; Loll, B.; Wahl, C.M.  
Deposited on : 2020-09-14  
Resolution : 4.30 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.dev133  
Mogul : 1.8.4, CSD as541be (2020)  
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) : 2.50

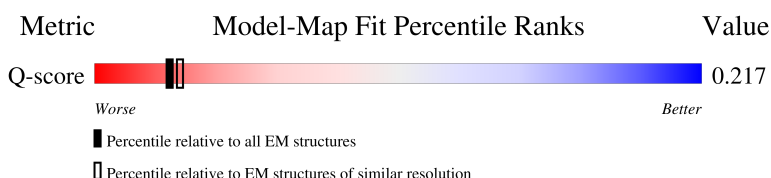
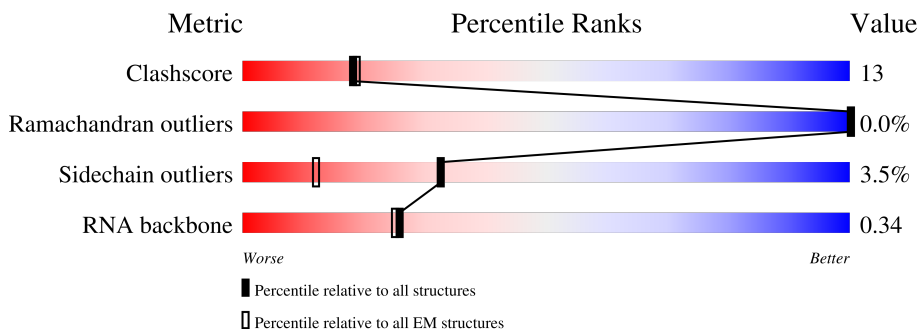
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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                       | 4585 ( 3.80 - 4.80 )                                     |

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     | 419    | <div> <div>12%</div> <div>61%</div> <div>36%</div> <div>.</div> </div> |
| 1   | b     | 419    | <div> <div>5%</div> <div>61%</div> <div>37%</div> <div>.</div> </div>  |
| 1   | c     | 419    | <div> <div>5%</div> <div>62%</div> <div>36%</div> <div>.</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | d     | 419    |                  |
| 1   | e     | 419    |                  |
| 1   | f     | 419    |                  |
| 2   | A     | 497    |                  |
| 3   | U     | 329    |                  |
| 3   | V     | 329    |                  |
| 4   | W     | 91     |                  |
| 5   | X     | 1342   |                  |
| 6   | Y     | 1416   |                  |
| 7   | K     | 50     |                  |
| 8   | L     | 50     |                  |
| 9   | R     | 99     |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 12  | BEF  | b     | 1002 | -         | -        | X       | -                |
| 12  | BEF  | c     | 503  | -         | -        | X       | -                |
| 12  | BEF  | c     | 504  | -         | -        | X       | -                |
| 12  | BEF  | e     | 1002 | -         | -        | X       | -                |

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 51610 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 Transcription termination factor Rho.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | f     | 417      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3280  | 2065 | 581 | 617 | 17 |         |       |
| 1   | a     | 417      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3280  | 2065 | 581 | 617 | 17 |         |       |
| 1   | b     | 417      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3280  | 2065 | 581 | 617 | 17 |         |       |
| 1   | c     | 417      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3280  | 2065 | 581 | 617 | 17 |         |       |
| 1   | d     | 417      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3280  | 2065 | 581 | 617 | 17 |         |       |
| 1   | e     | 417      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3280  | 2065 | 581 | 617 | 17 |         |       |

- Molecule 2 is a protein called Transcription termination/antitermination protein NusA.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | A     | 495      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3852  | 2396 | 669 | 774 | 13 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -1      | GLY      | -      | expression tag | UNP C3SSN7 |
| A     | 0       | ALA      | -      | expression tag | UNP C3SSN7 |

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | U     | 235      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1825  | 1135 | 325 | 359 | 6 |         |       |
| 3   | V     | 321      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2504  | 1566 | 441 | 489 | 8 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | W     | 79       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 627   | 382 | 118 | 126 | 1 |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 5   | X     | 1340     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10567 | 6631 | 1841 | 2052 | 43 |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta'.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 6   | Y     | 1358     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10545 | 6620 | 1883 | 1992 | 50 |         |       |

There are 9 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| Y     | 1408    | LEU      | -      | expression tag | UNP C3SIA2 |
| Y     | 1409    | GLU      | -      | expression tag | UNP C3SIA2 |
| Y     | 1410    | VAL      | -      | expression tag | UNP C3SIA2 |
| Y     | 1411    | HIS      | -      | expression tag | UNP C3SIA2 |
| Y     | 1412    | HIS      | -      | expression tag | UNP C3SIA2 |
| Y     | 1413    | HIS      | -      | expression tag | UNP C3SIA2 |
| Y     | 1414    | HIS      | -      | expression tag | UNP C3SIA2 |
| Y     | 1415    | HIS      | -      | expression tag | UNP C3SIA2 |
| Y     | 1416    | HIS      | -      | expression tag | UNP C3SIA2 |

- Molecule 7 is a DNA chain called ntDNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7   | K     | 26       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 538   | 254 | 103 | 155 | 26 |         |       |

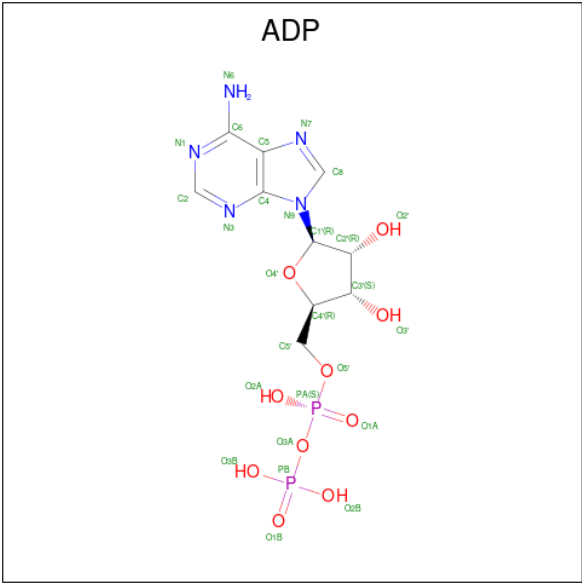
- Molecule 8 is a DNA chain called tDNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 8   | L     | 35       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 704   | 335 | 127 | 208 | 34 |         |       |

- Molecule 9 is a RNA chain called rut RNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 9   | R     | 28       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 590   | 264 | 103 | 195 | 28 |         |       |

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 10  | a     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 10  | b     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 10  | c     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 10  | d     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 10  | e     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

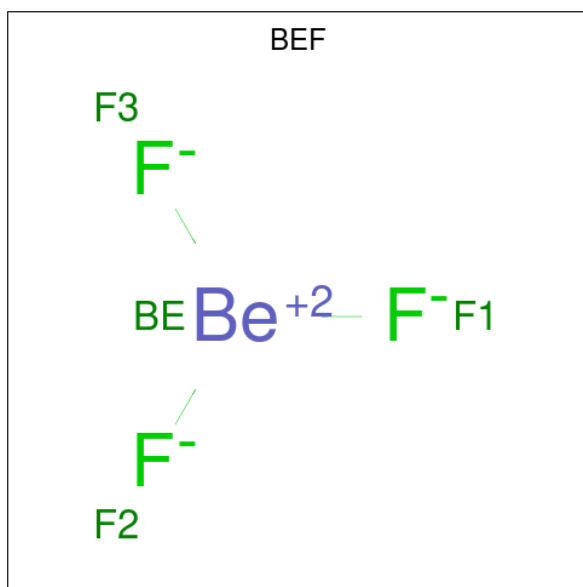
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 11  | a     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 11  | b     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 11  | c     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 11  | d     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 11  | e     | 1        | Total<br>1 | Mg<br>1 | 0       |
| 11  | Y     | 1        | Total<br>1 | Mg<br>1 | 0       |

- Molecule 12 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula:  $\text{BeF}_3$ ).



| Mol | Chain | Residues | Atoms      |         |        | AltConf |
|-----|-------|----------|------------|---------|--------|---------|
| 12  | a     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |
| 12  | b     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |
| 12  | c     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |
| 12  | c     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |
| 12  | e     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 13  | Y     | 2        | Total<br>2 | Zn<br>2 | 0       |

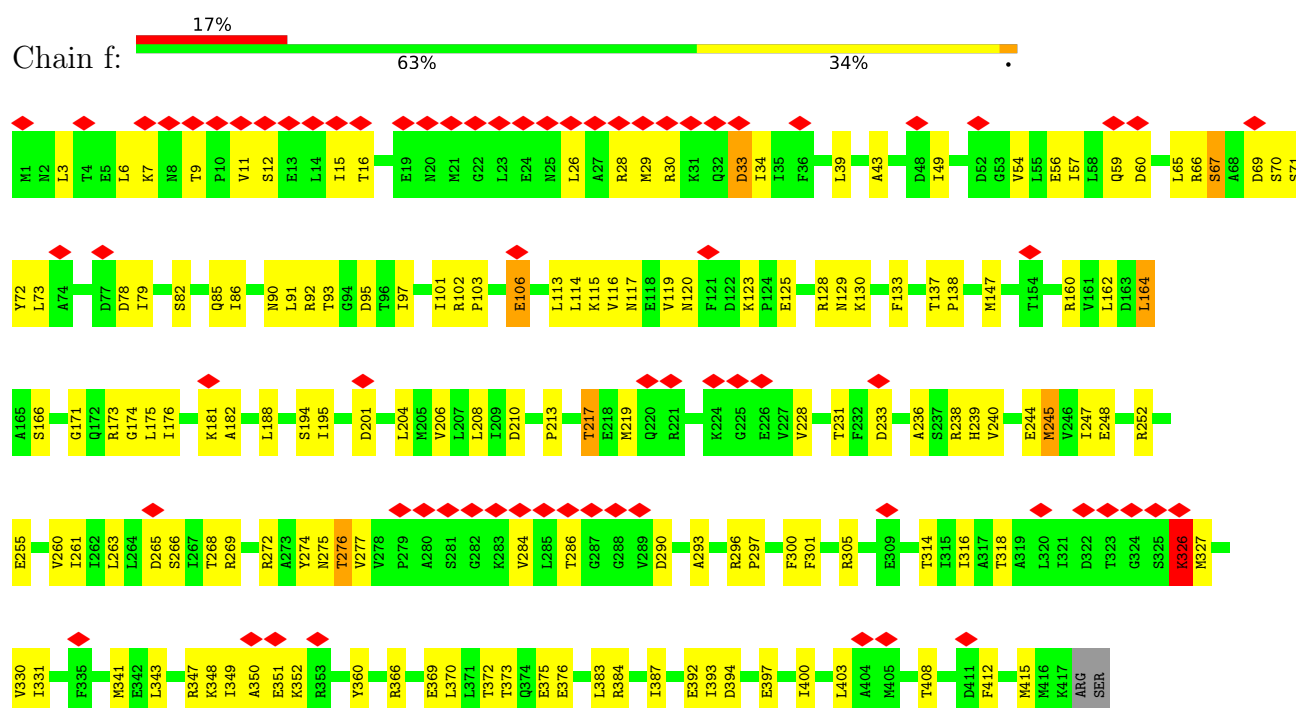
- Molecule 14 is water.

| Mol | Chain | Residues | Atoms      |        | AltConf |
|-----|-------|----------|------------|--------|---------|
| 14  | a     | 3        | Total<br>3 | O<br>3 | 0       |
| 14  | b     | 3        | Total<br>3 | O<br>3 | 0       |
| 14  | c     | 3        | Total<br>3 | O<br>3 | 0       |
| 14  | d     | 3        | Total<br>3 | O<br>3 | 0       |
| 14  | e     | 3        | Total<br>3 | O<br>3 | 0       |

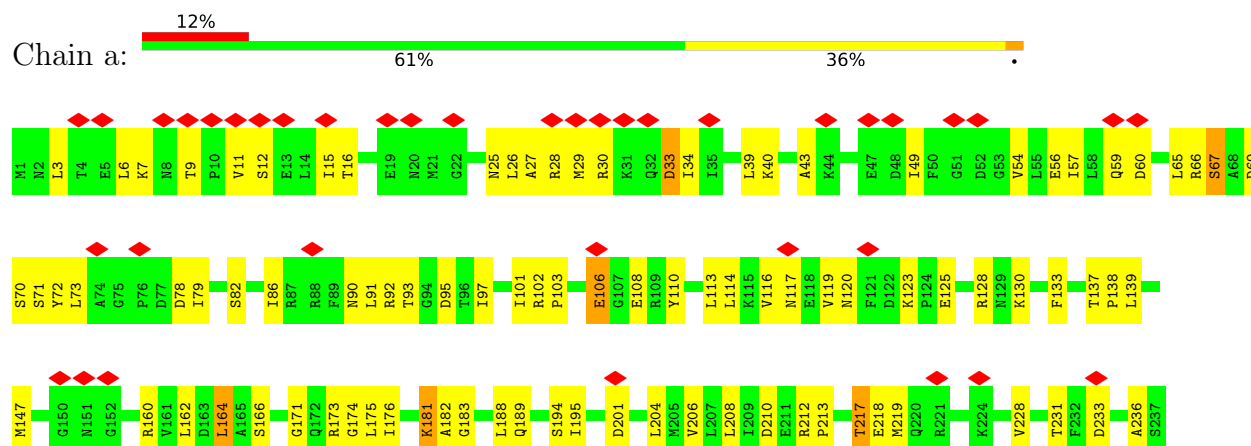
### 3 Residue-property plots

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: Transcription termination factor Rho



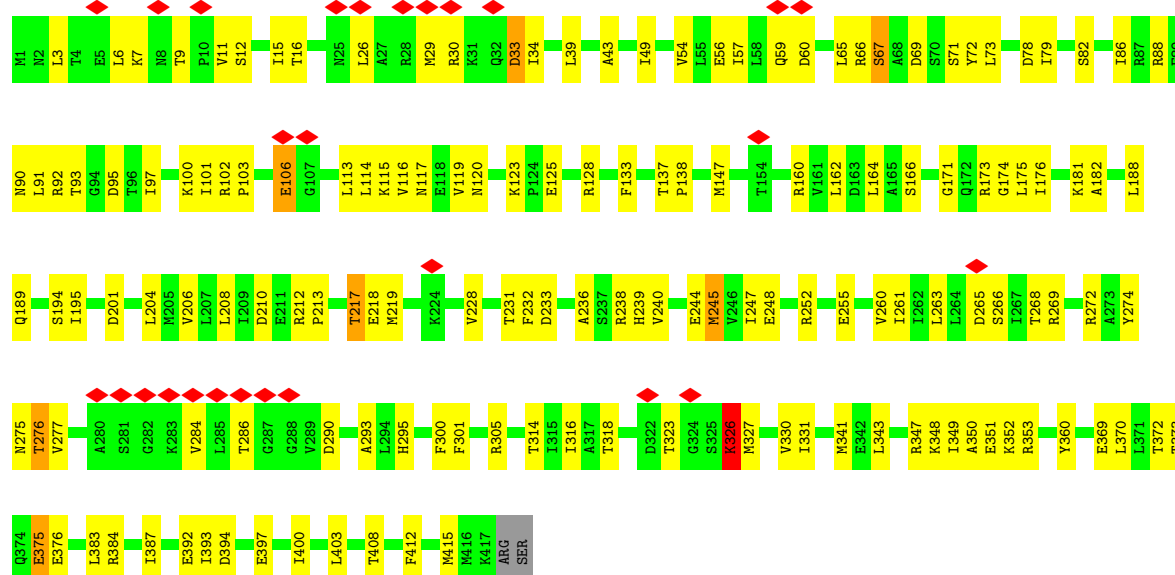
#### • Molecule 1: Transcription termination factor Rho







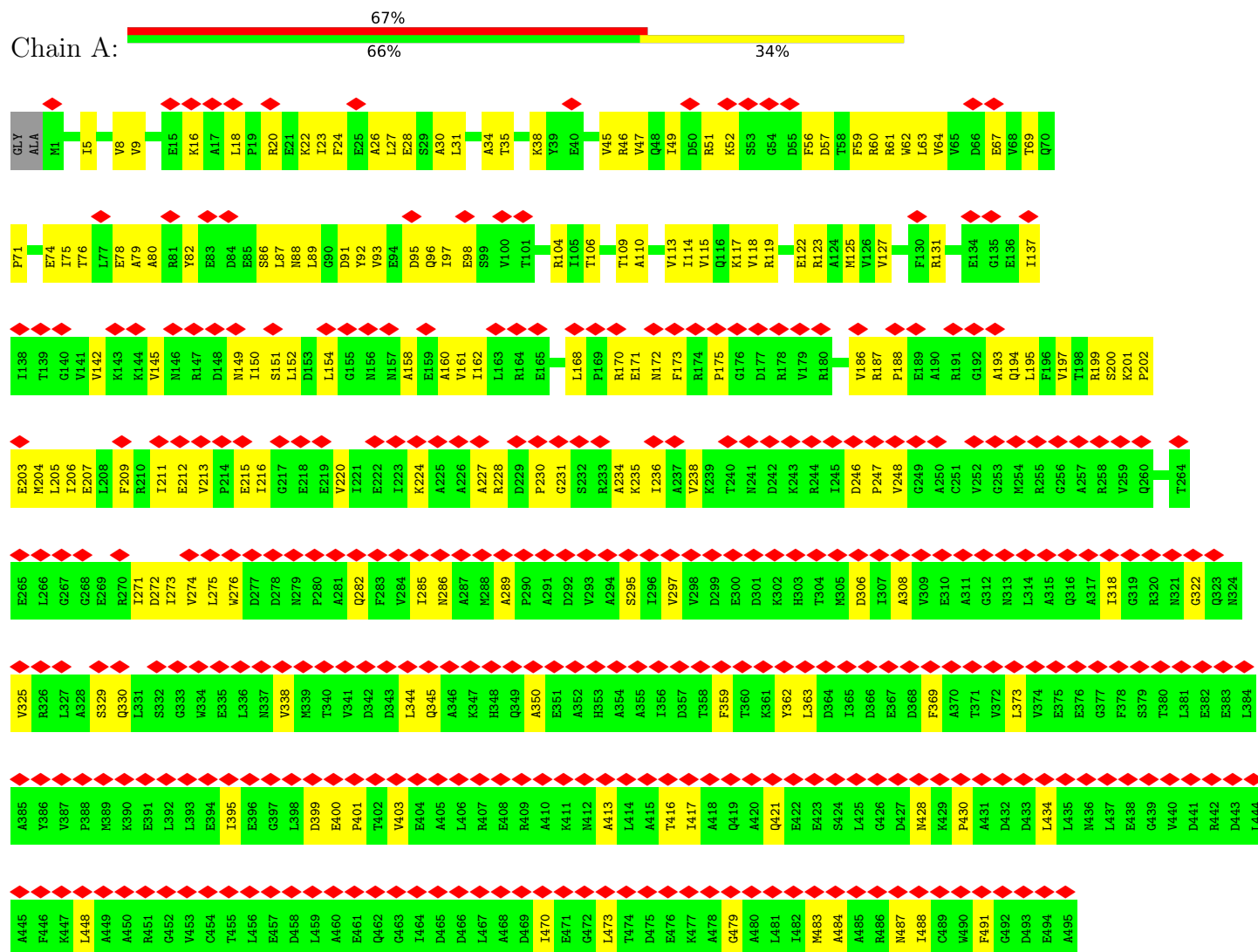
• Molecule 1: Transcription termination factor Rho



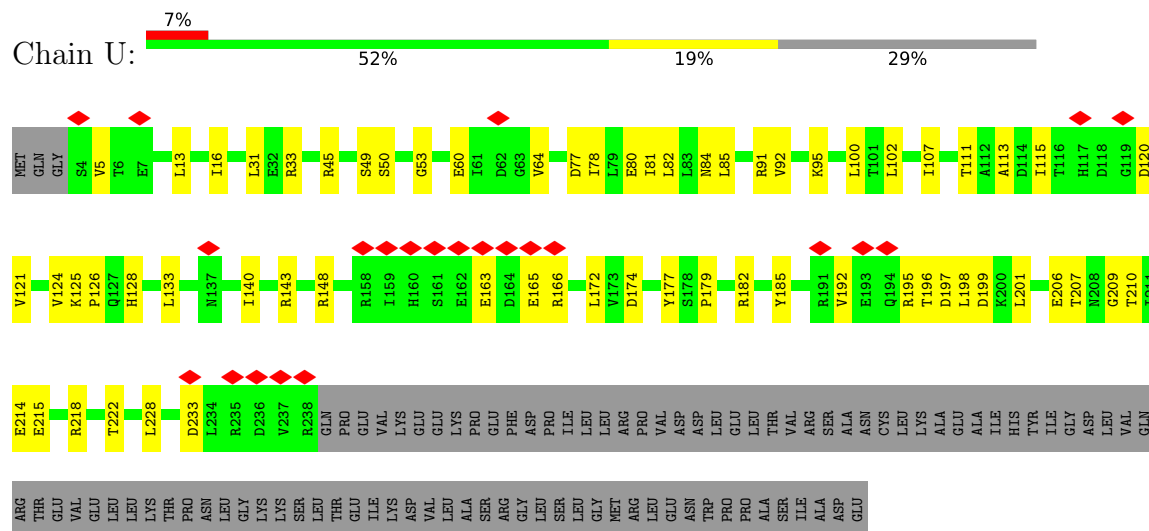
• Molecule 1: Transcription termination factor Rho



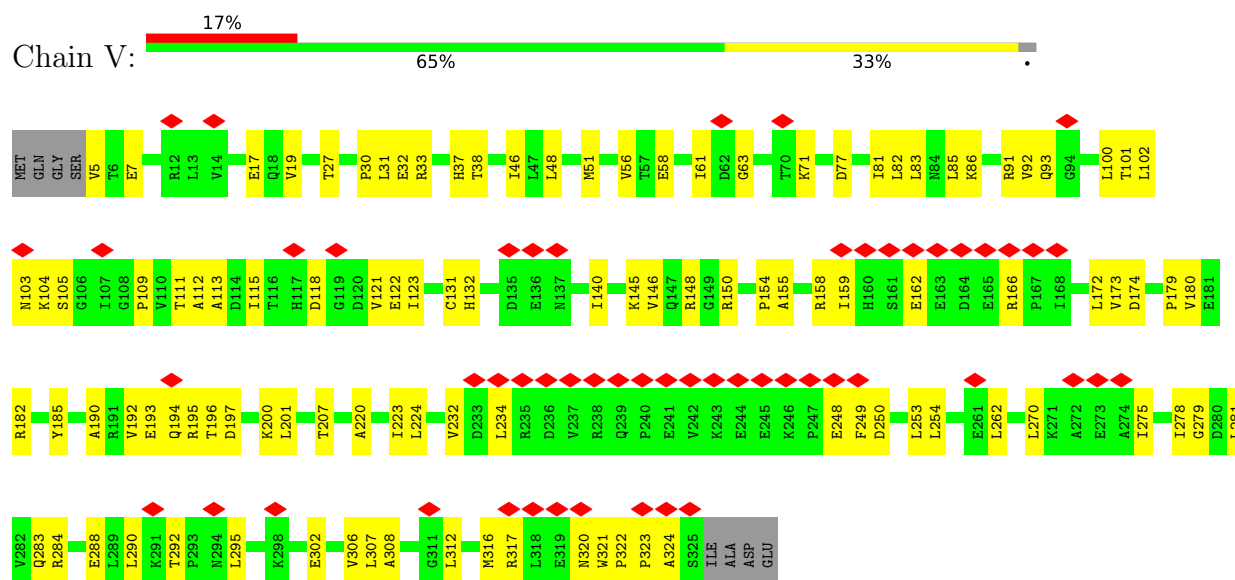
• Molecule 2: Transcription termination/antitermination protein NusA



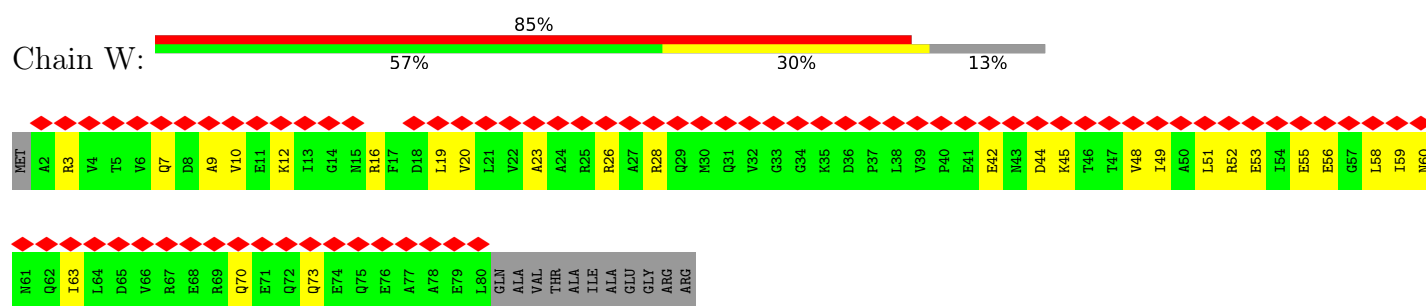
• Molecule 3: DNA-directed RNA polymerase subunit alpha



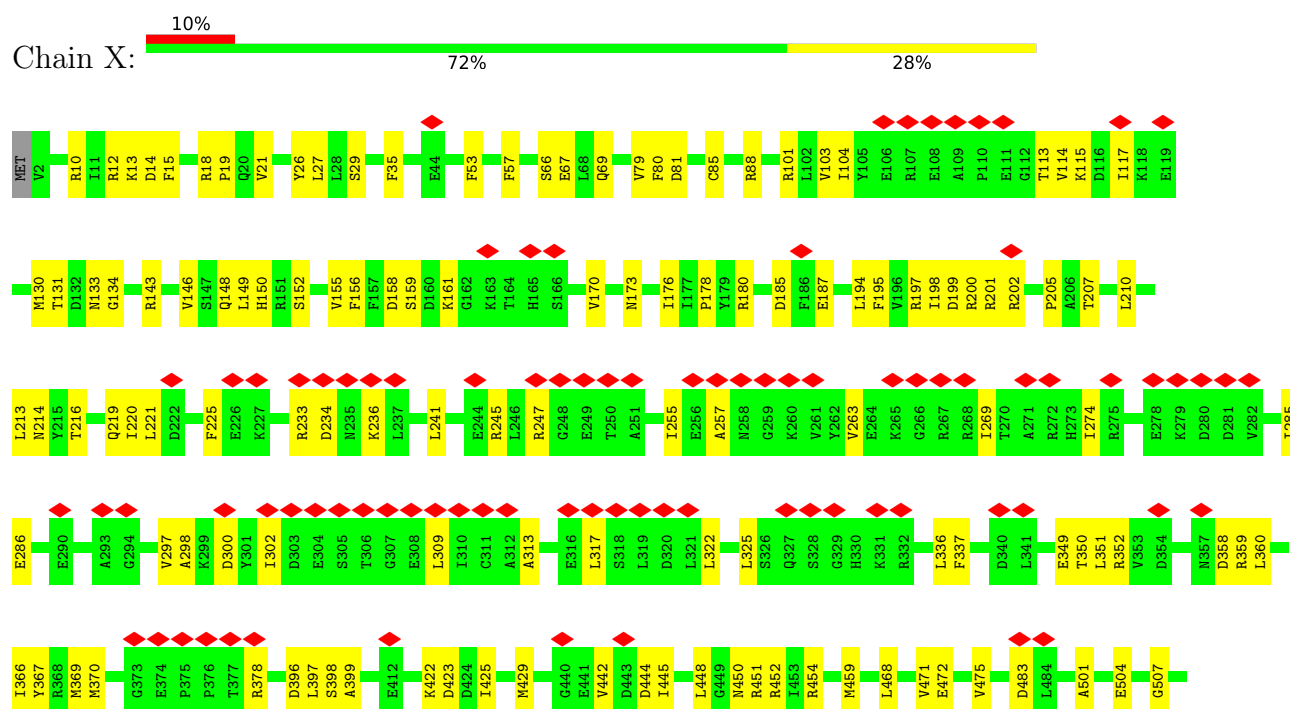
- Molecule 3: DNA-directed RNA polymerase subunit alpha

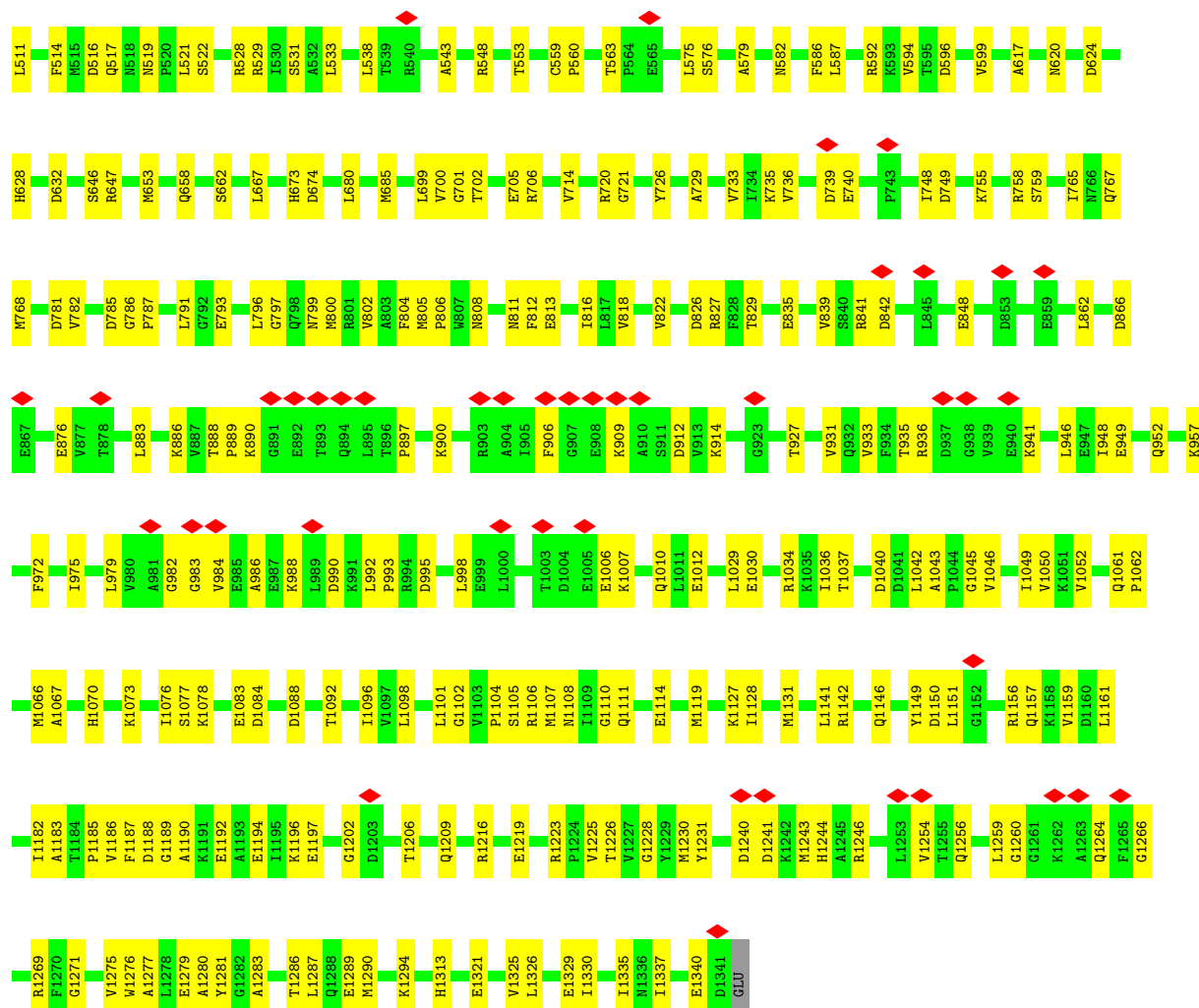


- Molecule 4: DNA-directed RNA polymerase subunit omega

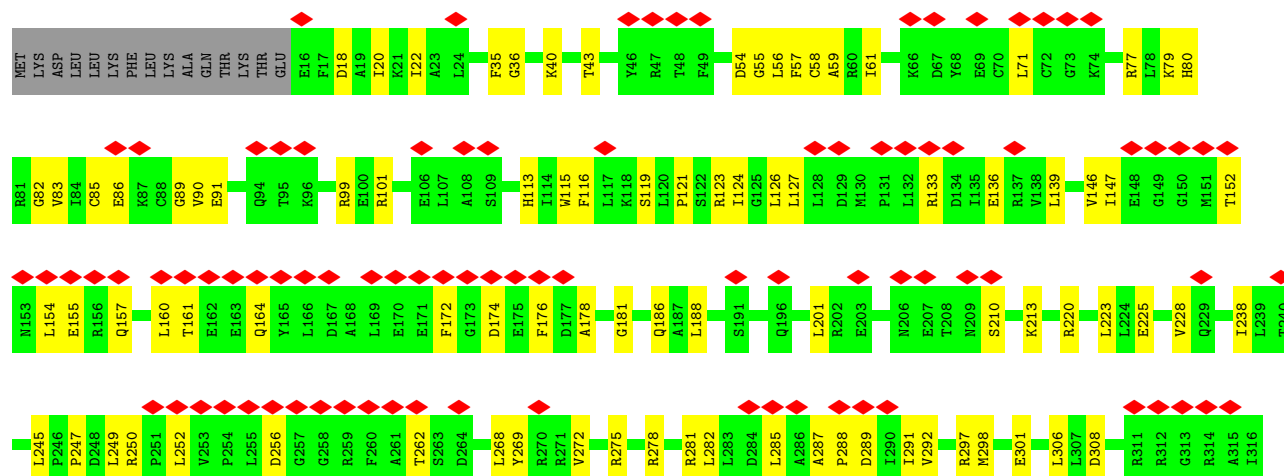


- Molecule 5: DNA-directed RNA polymerase subunit beta

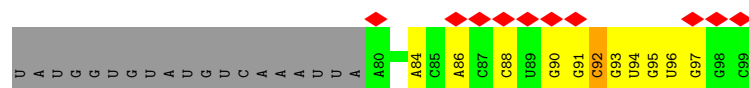




• Molecule 6: DNA-directed RNA polymerase subunit beta'







## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 40157                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI POLARA 300                          | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 8000                                    | Depositor |
| Maximum defocus (nm)                 | 25000                                   | Depositor |
| Magnification                        | 31000                                   | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.304                                   | Depositor |
| Minimum map value                    | 0.000                                   | Depositor |
| Average map value                    | 0.003                                   | Depositor |
| Map value standard deviation         | 0.017                                   | Depositor |
| Recommended contour level            | 0.11                                    | Depositor |
| Map size (Å)                         | 372.0, 372.0, 372.0                     | wwPDB     |
| Map dimensions                       | 300, 300, 300                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.24, 1.24, 1.24                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.12         | 0/3329      | 0.33        | 1/4483 (0.0%)  |
| 1   | b     | 0.12         | 0/3329      | 0.33        | 1/4483 (0.0%)  |
| 1   | c     | 0.12         | 0/3329      | 0.33        | 1/4483 (0.0%)  |
| 1   | d     | 0.12         | 0/3329      | 0.33        | 1/4483 (0.0%)  |
| 1   | e     | 0.12         | 0/3329      | 0.33        | 1/4483 (0.0%)  |
| 1   | f     | 0.12         | 0/3329      | 0.33        | 1/4483 (0.0%)  |
| 2   | A     | 0.11         | 0/3897      | 0.34        | 0/5273         |
| 3   | U     | 0.10         | 0/1847      | 0.30        | 0/2503         |
| 3   | V     | 0.11         | 0/2538      | 0.32        | 0/3441         |
| 4   | W     | 0.10         | 0/629       | 0.29        | 0/847          |
| 5   | X     | 0.11         | 0/10736     | 0.29        | 0/14487        |
| 6   | Y     | 0.10         | 0/10706     | 0.28        | 0/14456        |
| 7   | K     | 0.23         | 0/603       | 0.42        | 0/927          |
| 8   | L     | 0.21         | 0/786       | 0.57        | 2/1206 (0.2%)  |
| 9   | R     | 0.08         | 0/656       | 0.21        | 0/1016         |
| All | All   | 0.11         | 0/52372     | 0.32        | 8/71054 (0.0%) |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 8   | L     | 20  | DC   | OP2-P-O3' | -8.58 | 82.25       | 108.00   |
| 8   | L     | 20  | DC   | OP1-P-O3' | -7.89 | 84.32       | 108.00   |
| 1   | b     | 326 | LYS  | CB-CG-CD  | 5.04  | 122.88      | 111.30   |
| 1   | e     | 326 | LYS  | CB-CG-CD  | 5.04  | 122.88      | 111.30   |
| 1   | c     | 326 | LYS  | CB-CG-CD  | 5.03  | 122.87      | 111.30   |
| 1   | d     | 326 | LYS  | CB-CG-CD  | 5.03  | 122.87      | 111.30   |
| 1   | f     | 326 | LYS  | CB-CG-CD  | 5.02  | 122.85      | 111.30   |
| 1   | a     | 326 | LYS  | CB-CG-CD  | 5.01  | 122.83      | 111.30   |

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     | 3280  | 0        | 3358     | 107     | 0            |
| 1   | b     | 3280  | 0        | 3357     | 103     | 0            |
| 1   | c     | 3280  | 0        | 3357     | 106     | 0            |
| 1   | d     | 3280  | 0        | 3358     | 96      | 0            |
| 1   | e     | 3280  | 0        | 3359     | 97      | 0            |
| 1   | f     | 3280  | 0        | 3359     | 98      | 0            |
| 2   | A     | 3852  | 0        | 3835     | 120     | 0            |
| 3   | U     | 1825  | 0        | 1853     | 44      | 0            |
| 3   | V     | 2504  | 0        | 2558     | 74      | 0            |
| 4   | W     | 627   | 0        | 634      | 19      | 0            |
| 5   | X     | 10567 | 0        | 10585    | 278     | 0            |
| 6   | Y     | 10545 | 0        | 10761    | 284     | 0            |
| 7   | K     | 538   | 0        | 293      | 12      | 0            |
| 8   | L     | 704   | 0        | 394      | 24      | 0            |
| 9   | R     | 590   | 0        | 304      | 14      | 0            |
| 10  | a     | 27    | 0        | 12       | 2       | 0            |
| 10  | b     | 27    | 0        | 12       | 2       | 0            |
| 10  | c     | 27    | 0        | 12       | 1       | 0            |
| 10  | d     | 27    | 0        | 12       | 1       | 0            |
| 10  | e     | 27    | 0        | 12       | 3       | 0            |
| 11  | Y     | 1     | 0        | 0        | 0       | 0            |
| 11  | a     | 1     | 0        | 0        | 0       | 0            |
| 11  | b     | 1     | 0        | 0        | 0       | 0            |
| 11  | c     | 1     | 0        | 0        | 0       | 0            |
| 11  | d     | 1     | 0        | 0        | 0       | 0            |
| 11  | e     | 1     | 0        | 0        | 0       | 0            |
| 12  | a     | 4     | 0        | 0        | 1       | 0            |
| 12  | b     | 4     | 0        | 0        | 3       | 0            |
| 12  | c     | 8     | 0        | 0        | 4       | 0            |
| 12  | e     | 4     | 0        | 0        | 2       | 0            |
| 13  | Y     | 2     | 0        | 0        | 0       | 0            |
| 14  | a     | 3     | 0        | 0        | 0       | 0            |
| 14  | b     | 3     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14  | c     | 3     | 0        | 0        | 0       | 0            |
| 14  | d     | 3     | 0        | 0        | 0       | 0            |
| 14  | e     | 3     | 0        | 0        | 0       | 0            |
| All | All   | 51610 | 0        | 51425    | 1361    | 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 13.

All (1361) 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:173:ARG:O    | 1:a:341:MET:HB3   | 1.69                     | 0.93              |
| 1:e:173:ARG:O    | 1:e:341:MET:HB3   | 1.69                     | 0.93              |
| 1:f:173:ARG:O    | 1:f:341:MET:HB3   | 1.68                     | 0.93              |
| 1:d:173:ARG:O    | 1:d:341:MET:HB3   | 1.68                     | 0.93              |
| 1:c:173:ARG:O    | 1:c:341:MET:HB3   | 1.68                     | 0.92              |
| 1:b:173:ARG:O    | 1:b:341:MET:HB3   | 1.68                     | 0.91              |
| 3:V:158:ARG:HG3  | 3:V:172:LEU:HD13  | 1.58                     | 0.83              |
| 1:d:88:ARG:HH21  | 2:A:87:LEU:HA     | 1.44                     | 0.83              |
| 6:Y:362:ARG:H    | 6:Y:365:GLN:HE21  | 1.26                     | 0.82              |
| 1:d:43:ALA:HB1   | 1:d:103:PRO:HG3   | 1.64                     | 0.80              |
| 1:e:43:ALA:HB1   | 1:e:103:PRO:HG3   | 1.64                     | 0.79              |
| 1:a:43:ALA:HB1   | 1:a:103:PRO:HG3   | 1.64                     | 0.79              |
| 1:f:43:ALA:HB1   | 1:f:103:PRO:HG3   | 1.64                     | 0.78              |
| 1:b:43:ALA:HB1   | 1:b:103:PRO:HG3   | 1.64                     | 0.78              |
| 1:c:43:ALA:HB1   | 1:c:103:PRO:HG3   | 1.64                     | 0.77              |
| 4:W:3:ARG:HH12   | 4:W:55:GLU:HG3    | 1.51                     | 0.76              |
| 2:A:400:GLU:HG2  | 2:A:401:PRO:HD3   | 1.68                     | 0.74              |
| 5:X:1006:GLU:OE1 | 5:X:1010:GLN:NE2  | 2.21                     | 0.74              |
| 2:A:199:ARG:HG2  | 2:A:204:MET:HE2   | 1.68                     | 0.74              |
| 1:a:3:LEU:HD12   | 1:a:7:LYS:HE3     | 1.70                     | 0.74              |
| 1:f:3:LEU:HD12   | 1:f:7:LYS:HE3     | 1.70                     | 0.74              |
| 1:d:3:LEU:HD12   | 1:d:7:LYS:HE3     | 1.70                     | 0.74              |
| 5:X:425:ILE:HG22 | 5:X:429:MET:HE2   | 1.70                     | 0.73              |
| 1:e:3:LEU:HD12   | 1:e:7:LYS:HE3     | 1.70                     | 0.73              |
| 1:b:3:LEU:HD12   | 1:b:7:LYS:HE3     | 1.70                     | 0.73              |
| 6:Y:1075:ARG:HE  | 6:Y:1100:PHE:HB3  | 1.52                     | 0.73              |
| 1:c:3:LEU:HD12   | 1:c:7:LYS:HE3     | 1.70                     | 0.73              |
| 6:Y:527:LEU:HB2  | 6:Y:550:VAL:HG12  | 1.70                     | 0.73              |
| 6:Y:425:ARG:HG3  | 6:Y:427:PRO:HD2   | 1.70                     | 0.72              |
| 5:X:957:LYS:HE2  | 5:X:1029:LEU:HD11 | 1.70                     | 0.72              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:X:1157:GLN:HG3 | 5:X:1159:VAL:HG13 | 1.72                     | 0.72              |
| 1:a:59:GLN:NE2   | 1:a:60:ASP:OD1    | 2.24                     | 0.71              |
| 6:Y:586:GLY:HA3  | 6:Y:612:LEU:HD21  | 1.71                     | 0.71              |
| 1:f:59:GLN:NE2   | 1:f:60:ASP:OD1    | 2.24                     | 0.71              |
| 2:A:97:ILE:HG22  | 2:A:98:GLU:H      | 1.55                     | 0.71              |
| 1:d:59:GLN:NE2   | 1:d:60:ASP:OD1    | 2.24                     | 0.71              |
| 1:e:59:GLN:NE2   | 1:e:60:ASP:OD1    | 2.24                     | 0.71              |
| 1:f:90:ASN:HB3   | 1:a:28:ARG:HD3    | 1.72                     | 0.71              |
| 1:c:59:GLN:NE2   | 1:c:60:ASP:OD1    | 2.24                     | 0.70              |
| 2:A:49:ILE:HG23  | 2:A:56:PHE:HB3    | 1.71                     | 0.70              |
| 1:f:128:ARG:HG3  | 1:a:25:ASN:HD22   | 1.53                     | 0.70              |
| 1:b:59:GLN:NE2   | 1:b:60:ASP:OD1    | 2.24                     | 0.70              |
| 6:Y:790:THR:HG23 | 8:L:1:DT:H72      | 1.73                     | 0.70              |
| 2:A:26:ALA:HB2   | 2:A:117:LYS:HD3   | 1.73                     | 0.70              |
| 6:Y:527:LEU:HD23 | 6:Y:548:VAL:HG11  | 1.71                     | 0.70              |
| 1:f:115:LYS:HB3  | 9:R:19:C:H5       | 1.56                     | 0.70              |
| 1:e:326:LYS:HE3  | 1:e:326:LYS:HA    | 1.74                     | 0.70              |
| 1:f:326:LYS:HA   | 1:f:326:LYS:HE3   | 1.74                     | 0.69              |
| 6:Y:926:PRO:HG2  | 6:Y:1248:ILE:HD11 | 1.73                     | 0.69              |
| 1:a:326:LYS:HA   | 1:a:326:LYS:HE3   | 1.74                     | 0.69              |
| 1:b:326:LYS:HE3  | 1:b:326:LYS:HA    | 1.74                     | 0.69              |
| 1:d:326:LYS:HE3  | 1:d:326:LYS:HA    | 1.74                     | 0.69              |
| 6:Y:824:PRO:HD3  | 6:Y:835:LEU:HB2   | 1.74                     | 0.69              |
| 2:A:18:LEU:HA    | 2:A:22:LYS:HD2    | 1.75                     | 0.68              |
| 5:X:21:VAL:HG11  | 5:X:592:ARG:HD2   | 1.75                     | 0.68              |
| 5:X:528:ARG:NH2  | 5:X:576:SER:O     | 2.27                     | 0.68              |
| 1:c:385:LYS:NZ   | 1:d:352:LYS:O     | 2.27                     | 0.68              |
| 5:X:360:LEU:HD12 | 5:X:378:ARG:HD2   | 1.76                     | 0.68              |
| 1:c:326:LYS:HE3  | 1:c:326:LYS:HA    | 1.74                     | 0.68              |
| 1:c:174:GLY:HA3  | 1:c:316:ILE:HD13  | 1.76                     | 0.68              |
| 1:d:349:ILE:HD11 | 1:d:392:GLU:HG3   | 1.76                     | 0.68              |
| 5:X:936:ARG:NH2  | 5:X:1043:ALA:O    | 2.27                     | 0.68              |
| 5:X:936:ARG:HH21 | 5:X:1046:VAL:H    | 1.40                     | 0.67              |
| 1:c:88:ARG:HH22  | 5:X:998:LEU:HB3   | 1.60                     | 0.67              |
| 1:c:349:ILE:HD11 | 1:c:392:GLU:HG3   | 1.76                     | 0.67              |
| 1:d:174:GLY:HA3  | 1:d:316:ILE:HD13  | 1.76                     | 0.67              |
| 5:X:180:ARG:HB3  | 5:X:396:ASP:HB2   | 1.74                     | 0.67              |
| 1:a:174:GLY:HA3  | 1:a:316:ILE:HD13  | 1.76                     | 0.67              |
| 1:a:349:ILE:HD11 | 1:a:392:GLU:HG3   | 1.76                     | 0.67              |
| 1:e:349:ILE:HD11 | 1:e:392:GLU:HG3   | 1.76                     | 0.67              |
| 6:Y:82:GLY:HA2   | 6:Y:91:GLU:HG2    | 1.76                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:f:174:GLY:HA3   | 1:f:316:ILE:HD13  | 1.76                     | 0.67              |
| 1:a:106:GLU:OE1   | 1:a:106:GLU:N     | 2.28                     | 0.67              |
| 1:e:106:GLU:N     | 1:e:106:GLU:OE1   | 2.28                     | 0.67              |
| 1:e:102:ARG:NH1   | 1:e:103:PRO:O     | 2.28                     | 0.67              |
| 1:f:102:ARG:NH1   | 1:f:103:PRO:O     | 2.28                     | 0.66              |
| 1:b:212:ARG:NH2   | 12:b:1002:BEF:F1  | 2.18                     | 0.66              |
| 1:d:106:GLU:N     | 1:d:106:GLU:OE1   | 2.28                     | 0.66              |
| 1:c:106:GLU:OE1   | 1:c:106:GLU:N     | 2.28                     | 0.66              |
| 1:d:102:ARG:NH1   | 1:d:103:PRO:O     | 2.28                     | 0.66              |
| 3:V:321:TRP:HA    | 3:V:323:PRO:HD3   | 1.76                     | 0.66              |
| 6:Y:139:LEU:HA    | 6:Y:181:GLY:HA2   | 1.75                     | 0.66              |
| 1:c:102:ARG:NH1   | 1:c:103:PRO:O     | 2.28                     | 0.66              |
| 1:b:106:GLU:N     | 1:b:106:GLU:OE1   | 2.28                     | 0.66              |
| 3:V:109:PRO:HB3   | 3:V:132:HIS:HA    | 1.78                     | 0.66              |
| 6:Y:245:LEU:O     | 6:Y:250:ARG:NH2   | 2.28                     | 0.66              |
| 1:b:102:ARG:NH1   | 1:b:103:PRO:O     | 2.28                     | 0.66              |
| 1:b:349:ILE:HD11  | 1:b:392:GLU:HG3   | 1.76                     | 0.66              |
| 1:e:174:GLY:HA3   | 1:e:316:ILE:HD13  | 1.76                     | 0.66              |
| 1:f:106:GLU:OE1   | 1:f:106:GLU:N     | 2.28                     | 0.66              |
| 9:R:92:C:H2'      | 9:R:93:G:C8       | 2.31                     | 0.66              |
| 6:Y:282:LEU:HB2   | 6:Y:287:ALA:HB2   | 1.78                     | 0.65              |
| 1:f:349:ILE:HD11  | 1:f:392:GLU:HG3   | 1.77                     | 0.65              |
| 1:a:102:ARG:NH1   | 1:a:103:PRO:O     | 2.28                     | 0.65              |
| 5:X:161:LYS:HB3   | 5:X:170:VAL:HG23  | 1.78                     | 0.65              |
| 5:X:931:VAL:HG12  | 5:X:1052:VAL:HG12 | 1.78                     | 0.65              |
| 6:Y:576:ARG:HD3   | 6:Y:593:ASN:HA    | 1.78                     | 0.65              |
| 5:X:159:SER:HB2   | 5:X:442:VAL:HG11  | 1.78                     | 0.65              |
| 5:X:986:ALA:O     | 5:X:990:ASP:HB2   | 1.97                     | 0.65              |
| 5:X:1337:ILE:HD12 | 6:Y:20:ILE:HD11   | 1.78                     | 0.65              |
| 1:b:174:GLY:HA3   | 1:b:316:ILE:HD13  | 1.76                     | 0.65              |
| 3:V:61:ILE:HG22   | 3:V:63:GLY:H      | 1.62                     | 0.65              |
| 6:Y:809:VAL:HG13  | 6:Y:912:GLY:H     | 1.60                     | 0.65              |
| 5:X:729:ALA:O     | 5:X:755:LYS:NZ    | 2.24                     | 0.65              |
| 6:Y:582:ILE:HD12  | 6:Y:623:GLN:HB3   | 1.79                     | 0.65              |
| 6:Y:746:LEU:HD23  | 6:Y:758:PRO:HB3   | 1.78                     | 0.65              |
| 2:A:199:ARG:HB3   | 2:A:204:MET:HG2   | 1.79                     | 0.65              |
| 5:X:1127:LYS:HE2  | 5:X:1202:GLY:HA2  | 1.78                     | 0.65              |
| 5:X:808:ASN:H     | 6:Y:633:ALA:HB2   | 1.63                     | 0.64              |
| 5:X:632:ASP:OD1   | 5:X:647:ARG:NE    | 2.28                     | 0.64              |
| 1:a:12:SER:O      | 1:a:16:THR:HG23   | 1.98                     | 0.64              |
| 1:d:12:SER:O      | 1:d:16:THR:HG23   | 1.98                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:A:487:ASN:HA   | 2:A:491:PHE:HB2   | 1.79                     | 0.64              |
| 6:Y:1321:SER:HA  | 6:Y:1348:LYS:HZ2  | 1.62                     | 0.64              |
| 2:A:297:VAL:HB   | 2:A:306:ASP:HB2   | 1.79                     | 0.64              |
| 1:d:176:ILE:HB   | 1:d:318:THR:HA    | 1.80                     | 0.64              |
| 5:X:890:LYS:HB3  | 5:X:914:LYS:HE2   | 1.80                     | 0.64              |
| 1:f:176:ILE:HB   | 1:f:318:THR:HA    | 1.80                     | 0.63              |
| 5:X:18:ARG:O     | 5:X:1156:ARG:NH1  | 2.31                     | 0.63              |
| 6:Y:794:GLY:HA3  | 8:L:1:DT:H1'      | 1.80                     | 0.63              |
| 8:L:19:DG:H2'    | 8:L:20:DC:C2      | 2.33                     | 0.63              |
| 1:c:12:SER:O     | 1:c:16:THR:HG23   | 1.98                     | 0.63              |
| 1:e:176:ILE:HB   | 1:e:318:THR:HA    | 1.80                     | 0.63              |
| 6:Y:945:ALA:HB3  | 6:Y:1022:PRO:HA   | 1.81                     | 0.63              |
| 3:V:162:GLU:HG2  | 3:V:166:ARG:HB3   | 1.78                     | 0.63              |
| 1:b:176:ILE:HB   | 1:b:318:THR:HA    | 1.80                     | 0.63              |
| 1:c:176:ILE:HB   | 1:c:318:THR:HA    | 1.80                     | 0.63              |
| 1:f:12:SER:O     | 1:f:16:THR:HG23   | 1.98                     | 0.63              |
| 5:X:813:GLU:OE2  | 6:Y:461:PHE:N     | 2.30                     | 0.63              |
| 1:b:385:LYS:NZ   | 1:c:352:LYS:O     | 2.32                     | 0.62              |
| 1:e:138:PRO:HG3  | 1:e:305:ARG:HD3   | 1.81                     | 0.62              |
| 3:V:83:LEU:HG    | 6:Y:528:THR:HG22  | 1.81                     | 0.62              |
| 1:b:208:LEU:HD11 | 1:b:219:MET:HG3   | 1.81                     | 0.62              |
| 4:W:53:GLU:HB3   | 4:W:59:ILE:HD12   | 1.81                     | 0.62              |
| 1:e:12:SER:O     | 1:e:16:THR:HG23   | 1.98                     | 0.62              |
| 1:e:208:LEU:HD11 | 1:e:219:MET:HG3   | 1.81                     | 0.62              |
| 5:X:521:LEU:HD12 | 5:X:667:LEU:HD12  | 1.81                     | 0.62              |
| 5:X:935:THR:HG21 | 5:X:941:LYS:HG2   | 1.81                     | 0.62              |
| 1:b:12:SER:O     | 1:b:16:THR:HG23   | 1.98                     | 0.62              |
| 1:d:208:LEU:HD11 | 1:d:219:MET:HG3   | 1.82                     | 0.62              |
| 2:A:479:GLY:O    | 2:A:483:MET:HG2   | 1.98                     | 0.62              |
| 6:Y:1000:GLY:HA3 | 6:Y:1026:PRO:HG3  | 1.81                     | 0.62              |
| 1:a:208:LEU:HD11 | 1:a:219:MET:HG3   | 1.81                     | 0.62              |
| 2:A:59:PHE:O     | 2:A:96:GLN:NE2    | 2.32                     | 0.62              |
| 5:X:131:THR:HG23 | 5:X:133:ASN:H     | 1.65                     | 0.62              |
| 1:c:138:PRO:HG3  | 1:c:305:ARG:HD3   | 1.82                     | 0.62              |
| 2:A:137:ILE:HD12 | 2:A:211:ILE:HD12  | 1.82                     | 0.62              |
| 3:V:162:GLU:HB2  | 3:V:172:LEU:HD11  | 1.80                     | 0.62              |
| 5:X:1279:GLU:HG2 | 6:Y:1347:LEU:HD21 | 1.80                     | 0.62              |
| 1:b:138:PRO:HG3  | 1:b:305:ARG:HD3   | 1.82                     | 0.62              |
| 6:Y:933:ARG:NH2  | 6:Y:934:THR:O     | 2.33                     | 0.62              |
| 1:f:138:PRO:HG3  | 1:f:305:ARG:HD3   | 1.82                     | 0.61              |
| 1:a:67:SER:OG    | 1:a:69:ASP:OD1    | 2.18                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:a:138:PRO:HG3  | 1:a:305:ARG:HD3   | 1.81                     | 0.61              |
| 1:a:176:ILE:HB   | 1:a:318:THR:HA    | 1.80                     | 0.61              |
| 5:X:1185:PRO:HD2 | 5:X:1189:GLY:HA2  | 1.80                     | 0.61              |
| 6:Y:77:ARG:HG3   | 6:Y:79:LYS:H      | 1.65                     | 0.61              |
| 8:L:4:DC:H2'     | 8:L:5:DA:C8       | 2.35                     | 0.61              |
| 5:X:26:TYR:HB3   | 5:X:29:SER:HB3    | 1.81                     | 0.61              |
| 5:X:700:VAL:HG21 | 5:X:1114:GLU:HG3  | 1.82                     | 0.61              |
| 6:Y:245:LEU:HD11 | 6:Y:249:LEU:HD22  | 1.82                     | 0.61              |
| 1:f:208:LEU:HD11 | 1:f:219:MET:HG3   | 1.81                     | 0.61              |
| 1:c:67:SER:OG    | 1:c:69:ASP:OD1    | 2.18                     | 0.61              |
| 2:A:363:LEU:HD23 | 2:A:369:PHE:HB2   | 1.82                     | 0.61              |
| 1:d:67:SER:OG    | 1:d:69:ASP:OD1    | 2.18                     | 0.61              |
| 1:d:138:PRO:HG3  | 1:d:305:ARG:HD3   | 1.81                     | 0.61              |
| 3:U:33:ARG:HH11  | 3:U:197:ASP:HB2   | 1.65                     | 0.61              |
| 2:A:104:ARG:NH1  | 5:X:862:LEU:O     | 2.34                     | 0.61              |
| 3:V:101:THR:OG1  | 3:V:103:ASN:OD1   | 2.19                     | 0.61              |
| 6:Y:972:LYS:HE2  | 6:Y:1002:VAL:HG13 | 1.82                     | 0.61              |
| 1:a:272:ARG:O    | 1:a:276:THR:HG22  | 2.01                     | 0.61              |
| 1:d:272:ARG:O    | 1:d:276:THR:HG22  | 2.01                     | 0.61              |
| 2:A:484:ALA:O    | 2:A:488:ILE:HG12  | 2.01                     | 0.61              |
| 5:X:517:GLN:HB3  | 5:X:759:SER:HB2   | 1.82                     | 0.61              |
| 1:f:129:ASN:HB2  | 1:a:25:ASN:HD21   | 1.64                     | 0.61              |
| 1:c:212:ARG:NH2  | 12:c:503:BEF:F1   | 2.24                     | 0.61              |
| 3:U:80:GLU:O     | 3:U:84:ASN:ND2    | 2.34                     | 0.61              |
| 1:f:67:SER:OG    | 1:f:69:ASP:OD1    | 2.18                     | 0.60              |
| 3:V:104:LYS:NZ   | 3:V:105:SER:O     | 2.33                     | 0.60              |
| 2:A:215:GLU:HB3  | 2:A:220:VAL:HG21  | 1.82                     | 0.60              |
| 6:Y:1367:GLN:HG2 | 6:Y:1371:ARG:HE   | 1.65                     | 0.60              |
| 1:b:67:SER:OG    | 1:b:69:ASP:OD1    | 2.18                     | 0.60              |
| 1:e:272:ARG:O    | 1:e:276:THR:HG22  | 2.01                     | 0.60              |
| 2:A:28:GLU:HG2   | 2:A:47:VAL:HB     | 1.84                     | 0.60              |
| 3:U:100:LEU:HD21 | 3:U:121:VAL:HG11  | 1.83                     | 0.60              |
| 5:X:103:VAL:HB   | 5:X:114:VAL:HG21  | 1.83                     | 0.60              |
| 6:Y:1178:THR:HA  | 6:Y:1184:ASP:HB3  | 1.83                     | 0.60              |
| 1:f:244:GLU:OE2  | 1:f:274:TYR:OH    | 2.12                     | 0.60              |
| 1:a:123:LYS:HG2  | 1:a:125:GLU:H     | 1.67                     | 0.60              |
| 3:U:95:LYS:NZ    | 3:U:120:ASP:OD2   | 2.34                     | 0.60              |
| 3:U:100:LEU:HD11 | 3:U:121:VAL:HG21  | 1.83                     | 0.60              |
| 1:e:67:SER:OG    | 1:e:69:ASP:OD1    | 2.18                     | 0.60              |
| 6:Y:791:ALA:HA   | 8:L:1:DT:C6       | 2.37                     | 0.60              |
| 1:c:208:LEU:HD11 | 1:c:219:MET:HG3   | 1.81                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:168:LEU:HB2   | 2:A:171:GLU:HB2   | 1.82                     | 0.60              |
| 5:X:933:VAL:HG12  | 5:X:1050:VAL:HG22 | 1.84                     | 0.60              |
| 1:e:244:GLU:OE2   | 1:e:274:TYR:OH    | 2.11                     | 0.60              |
| 3:U:222:THR:HA    | 3:V:232:VAL:HG23  | 1.83                     | 0.60              |
| 3:V:283:GLN:NE2   | 3:V:316:MET:O     | 2.34                     | 0.60              |
| 1:f:272:ARG:O     | 1:f:276:THR:HG22  | 2.01                     | 0.60              |
| 1:d:263:LEU:HD13  | 1:d:316:ILE:HB    | 1.84                     | 0.60              |
| 1:e:123:LYS:HG2   | 1:e:125:GLU:H     | 1.67                     | 0.60              |
| 2:A:145:VAL:HA    | 2:A:150:ILE:HG22  | 1.84                     | 0.60              |
| 5:X:818:VAL:HG12  | 5:X:1096:ILE:HG12 | 1.84                     | 0.60              |
| 5:X:1142:ARG:NH1  | 5:X:1161:LEU:O    | 2.34                     | 0.60              |
| 12:c:504:BEF:F1   | 1:d:212:ARG:NH2   | 2.23                     | 0.60              |
| 1:d:123:LYS:HG2   | 1:d:125:GLU:H     | 1.67                     | 0.60              |
| 6:Y:152:THR:HG23  | 6:Y:154:LEU:H     | 1.66                     | 0.60              |
| 1:b:123:LYS:HG2   | 1:b:125:GLU:H     | 1.67                     | 0.59              |
| 1:c:272:ARG:O     | 1:c:276:THR:HG22  | 2.01                     | 0.59              |
| 1:d:138:PRO:HD2   | 1:e:217:THR:HG21  | 1.83                     | 0.59              |
| 5:X:1105:SER:HB3  | 6:Y:731:ARG:HG3   | 1.83                     | 0.59              |
| 5:X:1269:ARG:HA   | 6:Y:346:ARG:HA    | 1.83                     | 0.59              |
| 6:Y:1046:ILE:HG22 | 6:Y:1061:VAL:HG12 | 1.84                     | 0.59              |
| 6:Y:884:SER:HB2   | 6:Y:887:SER:HB3   | 1.85                     | 0.59              |
| 6:Y:885:VAL:N     | 6:Y:1254:GLU:OE1  | 2.36                     | 0.59              |
| 1:f:123:LYS:HG2   | 1:f:125:GLU:H     | 1.67                     | 0.59              |
| 1:a:263:LEU:HD13  | 1:a:316:ILE:HB    | 1.84                     | 0.59              |
| 1:b:272:ARG:O     | 1:b:276:THR:HG22  | 2.01                     | 0.59              |
| 6:Y:747:MET:HE2   | 6:Y:775:SER:HA    | 1.84                     | 0.59              |
| 1:c:263:LEU:HD13  | 1:c:316:ILE:HB    | 1.84                     | 0.59              |
| 2:A:235:LYS:HD3   | 2:A:272:ASP:HB2   | 1.84                     | 0.59              |
| 1:c:123:LYS:HG2   | 1:c:125:GLU:H     | 1.67                     | 0.59              |
| 6:Y:275:ARG:NH1   | 6:Y:298:MET:O     | 2.34                     | 0.59              |
| 4:W:20:VAL:HG23   | 6:Y:478:LEU:HG    | 1.84                     | 0.59              |
| 5:X:69:GLN:HB2    | 5:X:101:ARG:HB3   | 1.85                     | 0.59              |
| 5:X:758:ARG:NH1   | 5:X:759:SER:O     | 2.35                     | 0.59              |
| 5:X:1006:GLU:O    | 5:X:1010:GLN:NE2  | 2.36                     | 0.58              |
| 2:A:142:VAL:HG12  | 2:A:152:LEU:HG    | 1.84                     | 0.58              |
| 1:f:263:LEU:HD13  | 1:f:316:ILE:HB    | 1.84                     | 0.58              |
| 2:A:470:ILE:HB    | 2:A:473:LEU:HB3   | 1.85                     | 0.58              |
| 1:e:263:LEU:HD13  | 1:e:316:ILE:HB    | 1.84                     | 0.58              |
| 2:A:213:VAL:HG12  | 2:A:216:ILE:H     | 1.68                     | 0.58              |
| 6:Y:79:LYS:HD3    | 9:R:23:U:H4'      | 1.85                     | 0.58              |
| 6:Y:513:MET:HA    | 6:Y:544:LEU:HD21  | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:160:ALA:HA   | 2:A:195:LEU:HB2  | 1.85                     | 0.58              |
| 3:U:182:ARG:HG2  | 3:U:206:GLU:HB3  | 1.85                     | 0.58              |
| 6:Y:36:GLY:HA3   | 6:Y:61:ILE:HG12  | 1.85                     | 0.58              |
| 6:Y:985:ILE:HG12 | 6:Y:991:THR:HG22 | 1.86                     | 0.58              |
| 4:W:12:LYS:NZ    | 4:W:55:GLU:O     | 2.37                     | 0.58              |
| 3:U:60:GLU:HB3   | 3:U:143:ARG:HB2  | 1.86                     | 0.58              |
| 4:W:7:GLN:HA     | 4:W:10:VAL:HG22  | 1.85                     | 0.58              |
| 6:Y:576:ARG:NH1  | 6:Y:593:ASN:OD1  | 2.37                     | 0.58              |
| 1:e:93:THR:O     | 1:e:252:ARG:NH1  | 2.37                     | 0.58              |
| 6:Y:160:LEU:HD22 | 6:Y:164:GLN:HB3  | 1.85                     | 0.58              |
| 9:R:92:C:H2'     | 9:R:93:G:H8      | 1.69                     | 0.58              |
| 2:A:234:ALA:HB3  | 2:A:271:ILE:HG12 | 1.86                     | 0.57              |
| 6:Y:121:PRO:O    | 6:Y:123:ARG:NH1  | 2.36                     | 0.57              |
| 1:f:93:THR:O     | 1:f:252:ARG:NH1  | 2.37                     | 0.57              |
| 1:b:263:LEU:HD13 | 1:b:316:ILE:HB   | 1.84                     | 0.57              |
| 6:Y:437:PHE:HZ   | 6:Y:453:VAL:HG21 | 1.69                     | 0.57              |
| 1:a:188:LEU:HD22 | 1:a:263:LEU:HD12 | 1.87                     | 0.57              |
| 1:e:188:LEU:HD22 | 1:e:263:LEU:HD12 | 1.87                     | 0.57              |
| 2:A:161:VAL:HG11 | 2:A:193:ALA:HB1  | 1.86                     | 0.57              |
| 3:U:185:TYR:HB2  | 3:U:201:LEU:HD11 | 1.87                     | 0.57              |
| 5:X:202:ARG:HG3  | 5:X:369:MET:HE1  | 1.86                     | 0.57              |
| 1:d:93:THR:O     | 1:d:252:ARG:NH1  | 2.37                     | 0.57              |
| 3:V:86:LYS:HD2   | 3:V:174:ASP:HB2  | 1.85                     | 0.57              |
| 6:Y:43:THR:HA    | 6:Y:56:LEU:HB3   | 1.87                     | 0.57              |
| 6:Y:297:ARG:NH1  | 6:Y:301:GLU:OE2  | 2.38                     | 0.57              |
| 8:L:3:DC:H2'     | 8:L:4:DC:H6      | 1.70                     | 0.57              |
| 1:b:93:THR:O     | 1:b:252:ARG:NH1  | 2.37                     | 0.57              |
| 2:A:110:ALA:O    | 2:A:114:ILE:HG12 | 2.04                     | 0.57              |
| 2:A:186:VAL:HG12 | 2:A:188:PRO:HD3  | 1.86                     | 0.57              |
| 1:f:102:ARG:HE   | 9:R:22:A:H61     | 1.52                     | 0.57              |
| 1:a:66:ARG:NH1   | 1:a:78:ASP:OD2   | 2.38                     | 0.57              |
| 3:U:92:VAL:O     | 3:U:148:ARG:NH2  | 2.38                     | 0.57              |
| 4:W:48:VAL:HA    | 4:W:51:LEU:HD12  | 1.87                     | 0.57              |
| 5:X:12:ARG:NE    | 5:X:793:GLU:OE2  | 2.34                     | 0.57              |
| 5:X:714:VAL:HB   | 5:X:787:PRO:HD2  | 1.87                     | 0.57              |
| 1:f:138:PRO:HB3  | 1:f:305:ARG:HB2  | 1.87                     | 0.57              |
| 2:A:31:LEU:HB2   | 2:A:47:VAL:HG21  | 1.86                     | 0.57              |
| 5:X:103:VAL:HG12 | 5:X:117:ILE:HG12 | 1.87                     | 0.57              |
| 1:c:93:THR:O     | 1:c:252:ARG:NH1  | 2.37                     | 0.57              |
| 1:c:188:LEU:HD22 | 1:c:263:LEU:HD12 | 1.86                     | 0.57              |
| 1:d:66:ARG:NH1   | 1:d:78:ASP:OD2   | 2.38                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:V:194:GLN:HE21  | 6:Y:406:ALA:HB2   | 1.70                     | 0.57              |
| 5:X:841:ARG:HA    | 5:X:1046:VAL:HA   | 1.85                     | 0.57              |
| 1:c:115:LYS:HZ3   | 5:X:1012:GLU:CD   | 2.12                     | 0.57              |
| 6:Y:883:ARG:NH1   | 6:Y:898:CYS:SG    | 2.78                     | 0.57              |
| 1:b:66:ARG:NH1    | 1:b:78:ASP:OD2    | 2.38                     | 0.56              |
| 4:W:23:ALA:HB3    | 6:Y:478:LEU:HD21  | 1.87                     | 0.56              |
| 5:X:720:ARG:NH2   | 5:X:749:ASP:OD1   | 2.38                     | 0.56              |
| 5:X:941:LYS:NZ    | 5:X:1037:THR:O    | 2.37                     | 0.56              |
| 1:a:93:THR:O      | 1:a:252:ARG:NH1   | 2.37                     | 0.56              |
| 2:A:20:ARG:HH11   | 2:A:52:LYS:HE3    | 1.69                     | 0.56              |
| 5:X:143:ARG:NH1   | 5:X:507:GLY:O     | 2.38                     | 0.56              |
| 5:X:1119:MET:HE2  | 5:X:1228:GLY:HA2  | 1.86                     | 0.56              |
| 5:X:1283:ALA:HB1  | 5:X:1286:THR:HB   | 1.87                     | 0.56              |
| 6:Y:429:LEU:HD13  | 6:Y:925:GLU:HA    | 1.87                     | 0.56              |
| 8:L:18:DG:H2'     | 8:L:19:DG:OP1     | 2.05                     | 0.56              |
| 1:f:66:ARG:NH1    | 1:f:78:ASP:OD2    | 2.38                     | 0.56              |
| 1:f:160:ARG:HB3   | 1:f:403:LEU:HD11  | 1.88                     | 0.56              |
| 1:b:360:TYR:HE1   | 1:b:384:ARG:HG2   | 1.71                     | 0.56              |
| 1:c:360:TYR:HE1   | 1:c:384:ARG:HG2   | 1.71                     | 0.56              |
| 1:d:101:ILE:HG22  | 1:d:113:LEU:HA    | 1.87                     | 0.56              |
| 1:d:240:VAL:HG11  | 1:d:277:VAL:HG11  | 1.88                     | 0.56              |
| 2:A:171:GLU:OE1   | 2:A:199:ARG:NH2   | 2.39                     | 0.56              |
| 4:W:26:ARG:HD3    | 4:W:59:ILE:HD13   | 1.87                     | 0.56              |
| 5:X:1223:ARG:NH1  | 6:Y:719:PHE:O     | 2.38                     | 0.56              |
| 6:Y:519:ASN:ND2   | 6:Y:708:ASN:O     | 2.35                     | 0.56              |
| 6:Y:1002:VAL:HB   | 6:Y:1019:ASN:HB3  | 1.87                     | 0.56              |
| 6:Y:1218:HIS:NE2  | 6:Y:1306:LEU:O    | 2.38                     | 0.56              |
| 1:f:240:VAL:HG11  | 1:f:277:VAL:HG11  | 1.88                     | 0.56              |
| 1:a:138:PRO:HB3   | 1:a:305:ARG:HB2   | 1.87                     | 0.56              |
| 1:a:360:TYR:HE1   | 1:a:384:ARG:HG2   | 1.71                     | 0.56              |
| 1:b:101:ILE:HG22  | 1:b:113:LEU:HA    | 1.87                     | 0.56              |
| 1:c:240:VAL:HG11  | 1:c:277:VAL:HG11  | 1.88                     | 0.56              |
| 1:e:66:ARG:NH1    | 1:e:78:ASP:OD2    | 2.38                     | 0.56              |
| 5:X:1042:LEU:HD13 | 5:X:1049:ILE:HG13 | 1.87                     | 0.56              |
| 5:X:201:ARG:NH2   | 5:X:369:MET:O     | 2.39                     | 0.56              |
| 8:L:-1:DA:H2'     | 8:L:0:DA:C8       | 2.41                     | 0.56              |
| 1:f:128:ARG:HG3   | 1:a:25:ASN:ND2    | 2.20                     | 0.56              |
| 1:c:138:PRO:HB3   | 1:c:305:ARG:HB2   | 1.87                     | 0.56              |
| 3:V:51:MET:HG3    | 3:V:179:PRO:HD2   | 1.87                     | 0.56              |
| 2:A:34:ALA:HB1    | 2:A:106:THR:HG22  | 1.88                     | 0.56              |
| 6:Y:338:PHE:HB3   | 6:Y:1324:SER:HA   | 1.87                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:Y:418:GLU:HB3  | 6:Y:481:ARG:HH12  | 1.71                     | 0.56              |
| 1:a:240:VAL:HG11 | 1:a:277:VAL:HG11  | 1.88                     | 0.56              |
| 1:c:66:ARG:NH1   | 1:c:78:ASP:OD2    | 2.38                     | 0.56              |
| 1:c:95:ASP:OD1   | 1:c:120:ASN:ND2   | 2.30                     | 0.56              |
| 5:X:1128:ILE:HA  | 5:X:1131:MET:HE2  | 1.87                     | 0.56              |
| 1:b:188:LEU:HD22 | 1:b:263:LEU:HD12  | 1.87                     | 0.56              |
| 6:Y:1029:THR:HA  | 6:Y:1099:TYR:HE2  | 1.70                     | 0.56              |
| 1:b:337:GLY:HA3  | 1:c:269:ARG:HH22  | 1.71                     | 0.56              |
| 3:U:124:VAL:HG23 | 3:U:125:LYS:HG2   | 1.87                     | 0.56              |
| 6:Y:491:LEU:HB2  | 6:Y:904:ALA:HA    | 1.87                     | 0.56              |
| 1:f:188:LEU:HD22 | 1:f:263:LEU:HD12  | 1.87                     | 0.55              |
| 1:a:110:TYR:O    | 8:L:21:DC:N4      | 2.32                     | 0.55              |
| 1:a:116:VAL:HG21 | 1:a:119:VAL:HG23  | 1.89                     | 0.55              |
| 1:b:240:VAL:HG11 | 1:b:277:VAL:HG11  | 1.88                     | 0.55              |
| 3:V:91:ARG:HG3   | 3:V:122:GLU:HB3   | 1.87                     | 0.55              |
| 6:Y:268:LEU:HD13 | 6:Y:306:LEU:HA    | 1.87                     | 0.55              |
| 6:Y:326:SER:OG   | 6:Y:327:LEU:N     | 2.40                     | 0.55              |
| 1:a:101:ILE:HG22 | 1:a:113:LEU:HA    | 1.87                     | 0.55              |
| 1:c:160:ARG:HB3  | 1:c:403:LEU:HD11  | 1.88                     | 0.55              |
| 1:d:188:LEU:HD22 | 1:d:263:LEU:HD12  | 1.86                     | 0.55              |
| 1:e:138:PRO:HB3  | 1:e:305:ARG:HB2   | 1.87                     | 0.55              |
| 3:U:53:GLY:HA3   | 3:U:177:TYR:HB2   | 1.89                     | 0.55              |
| 5:X:201:ARG:HB3  | 5:X:369:MET:HE2   | 1.88                     | 0.55              |
| 5:X:1061:GLN:NE2 | 5:X:1240:ASP:OD1  | 2.38                     | 0.55              |
| 6:Y:1258:ARG:NH2 | 6:Y:1259:GLN:OE1  | 2.39                     | 0.55              |
| 1:c:88:ARG:NH2   | 5:X:998:LEU:HB3   | 2.21                     | 0.55              |
| 1:d:138:PRO:HB3  | 1:d:305:ARG:HB2   | 1.87                     | 0.55              |
| 1:d:360:TYR:HE1  | 1:d:384:ARG:HG2   | 1.71                     | 0.55              |
| 2:A:359:PHE:HB2  | 2:A:362:TYR:HB2   | 1.87                     | 0.55              |
| 3:V:180:VAL:O    | 6:Y:535:ARG:NH1   | 2.39                     | 0.55              |
| 5:X:1243:MET:HE3 | 6:Y:372:MET:HG3   | 1.88                     | 0.55              |
| 5:X:1321:GLU:O   | 5:X:1325:VAL:HG23 | 2.06                     | 0.55              |
| 1:a:160:ARG:HB3  | 1:a:403:LEU:HD11  | 1.88                     | 0.55              |
| 1:e:116:VAL:HG21 | 1:e:119:VAL:HG23  | 1.89                     | 0.55              |
| 3:V:185:TYR:HB2  | 3:V:201:LEU:HD11  | 1.88                     | 0.55              |
| 1:b:116:VAL:HG21 | 1:b:119:VAL:HG23  | 1.89                     | 0.55              |
| 1:b:138:PRO:HB3  | 1:b:305:ARG:HB2   | 1.87                     | 0.55              |
| 1:c:101:ILE:HG22 | 1:c:113:LEU:HA    | 1.87                     | 0.55              |
| 1:e:101:ILE:HG22 | 1:e:113:LEU:HA    | 1.87                     | 0.55              |
| 1:e:360:TYR:HE1  | 1:e:384:ARG:HG2   | 1.71                     | 0.55              |
| 2:A:71:PRO:HA    | 2:A:74:GLU:HB2    | 1.89                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:Y:147:ILE:HD13  | 6:Y:188:LEU:HD23 | 1.88                     | 0.55              |
| 1:b:132:LEU:HD11  | 1:c:28:ARG:O     | 2.05                     | 0.55              |
| 3:V:100:LEU:HD21  | 3:V:121:VAL:HG21 | 1.89                     | 0.55              |
| 3:V:292:THR:HB    | 3:V:295:LEU:HD12 | 1.88                     | 0.55              |
| 5:X:88:ARG:NH1    | 5:X:1040:ASP:OD2 | 2.38                     | 0.55              |
| 1:b:160:ARG:HB3   | 1:b:403:LEU:HD11 | 1.88                     | 0.55              |
| 10:b:1000:ADP:O1B | 12:b:1002:BEF:F2 | 2.14                     | 0.55              |
| 2:A:5:ILE:HA      | 2:A:8:VAL:HG12   | 1.87                     | 0.55              |
| 5:X:1223:ARG:HH12 | 6:Y:719:PHE:HD1  | 1.55                     | 0.55              |
| 5:X:1246:ARG:HH11 | 5:X:1266:GLY:HA2 | 1.71                     | 0.55              |
| 1:a:128:ARG:HG3   | 1:b:25:ASN:HD22  | 1.71                     | 0.55              |
| 1:e:160:ARG:HB3   | 1:e:403:LEU:HD11 | 1.88                     | 0.55              |
| 6:Y:797:THR:HG22  | 6:Y:924:GLY:HA3  | 1.89                     | 0.55              |
| 3:U:207:THR:HG23  | 3:U:209:GLY:H    | 1.71                     | 0.55              |
| 1:f:116:VAL:HG21  | 1:f:119:VAL:HG23 | 1.89                     | 0.54              |
| 5:X:18:ARG:NH2    | 5:X:620:ASN:O    | 2.40                     | 0.54              |
| 5:X:982:GLY:H     | 5:X:1007:LYS:HZ1 | 1.55                     | 0.54              |
| 6:Y:709:ARG:NH1   | 6:Y:710:ASP:OD2  | 2.39                     | 0.54              |
| 6:Y:962:ASN:ND2   | 6:Y:979:ASN:O    | 2.40                     | 0.54              |
| 6:Y:975:ILE:HG22  | 6:Y:977:SER:H    | 1.70                     | 0.54              |
| 1:f:101:ILE:HG22  | 1:f:113:LEU:HA   | 1.87                     | 0.54              |
| 1:f:360:TYR:HE1   | 1:f:384:ARG:HG2  | 1.71                     | 0.54              |
| 1:d:160:ARG:HB3   | 1:d:403:LEU:HD11 | 1.88                     | 0.54              |
| 6:Y:116:PHE:HB3   | 6:Y:124:ILE:HG13 | 1.88                     | 0.54              |
| 8:L:3:DC:H2'      | 8:L:4:DC:C6      | 2.42                     | 0.54              |
| 1:b:95:ASP:OD1    | 1:b:120:ASN:ND2  | 2.29                     | 0.54              |
| 1:e:240:VAL:HG11  | 1:e:277:VAL:HG11 | 1.88                     | 0.54              |
| 3:U:5:VAL:O       | 3:V:150:ARG:NH2  | 2.41                     | 0.54              |
| 5:X:113:THR:OG1   | 5:X:115:LYS:NZ   | 2.41                     | 0.54              |
| 6:Y:658:GLU:O     | 6:Y:659:ALA:C    | 2.50                     | 0.54              |
| 1:f:130:LYS:H     | 1:a:27:ALA:HB1   | 1.72                     | 0.54              |
| 1:d:86:ILE:HA     | 1:d:91:LEU:HD13  | 1.90                     | 0.54              |
| 1:d:116:VAL:HG21  | 1:d:119:VAL:HG23 | 1.89                     | 0.54              |
| 5:X:448:LEU:H     | 5:X:553:THR:HG21 | 1.72                     | 0.54              |
| 6:Y:1316:THR:HG22 | 6:Y:1318:SER:H   | 1.73                     | 0.54              |
| 1:e:86:ILE:HA     | 1:e:91:LEU:HD13  | 1.90                     | 0.54              |
| 1:e:171:GLY:N     | 1:e:314:THR:OG1  | 2.39                     | 0.54              |
| 3:U:13:LEU:HD11   | 3:U:16:ILE:HD11  | 1.89                     | 0.54              |
| 3:U:107:ILE:HA    | 3:U:133:LEU:O    | 2.08                     | 0.54              |
| 3:V:85:LEU:HD11   | 3:V:173:VAL:HG11 | 1.89                     | 0.54              |
| 6:Y:1045:THR:HG21 | 6:Y:1076:PRO:HD3 | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:X:699:LEU:HG    | 5:X:799:ASN:HD22  | 1.71                     | 0.54              |
| 1:d:72:TYR:HB3    | 1:d:245:MET:HE1   | 1.90                     | 0.54              |
| 1:c:337:GLY:HA3   | 1:d:269:ARG:HH22  | 1.71                     | 0.54              |
| 5:X:538:LEU:HD21  | 5:X:543:ALA:HA    | 1.90                     | 0.54              |
| 5:X:808:ASN:HD21  | 5:X:1216:ARG:HH22 | 1.55                     | 0.54              |
| 5:X:839:VAL:O     | 5:X:886:LYS:NZ    | 2.36                     | 0.54              |
| 1:b:49:ILE:HB     | 1:b:101:ILE:HG13  | 1.90                     | 0.54              |
| 5:X:180:ARG:NH2   | 5:X:396:ASP:OD2   | 2.40                     | 0.54              |
| 5:X:519:ASN:HB3   | 5:X:522:SER:HB3   | 1.89                     | 0.54              |
| 5:X:624:ASP:N     | 5:X:628:HIS:O     | 2.32                     | 0.54              |
| 6:Y:1036:ARG:HH22 | 6:Y:1085:GLY:HA2  | 1.72                     | 0.54              |
| 1:b:86:ILE:HA     | 1:b:91:LEU:HD13   | 1.90                     | 0.53              |
| 1:c:116:VAL:HG21  | 1:c:119:VAL:HG23  | 1.89                     | 0.53              |
| 1:c:213:PRO:O     | 1:c:217:THR:HG23  | 2.08                     | 0.53              |
| 1:e:72:TYR:HB3    | 1:e:245:MET:HE1   | 1.90                     | 0.53              |
| 2:A:82:TYR:HB3    | 3:V:290:LEU:HD12  | 1.88                     | 0.53              |
| 5:X:1062:PRO:HG3  | 5:X:1078:LYS:HA   | 1.90                     | 0.53              |
| 6:Y:960:LEU:HD11  | 6:Y:980:THR:HB    | 1.88                     | 0.53              |
| 1:a:86:ILE:HA     | 1:a:91:LEU:HD13   | 1.90                     | 0.53              |
| 1:e:49:ILE:HB     | 1:e:101:ILE:HG13  | 1.90                     | 0.53              |
| 6:Y:1044:GLN:NE2  | 6:Y:1070:GLY:O    | 2.39                     | 0.53              |
| 1:f:72:TYR:HB3    | 1:f:245:MET:HE1   | 1.90                     | 0.53              |
| 1:b:72:TYR:HB3    | 1:b:245:MET:HE1   | 1.90                     | 0.53              |
| 3:V:56:VAL:HA     | 3:V:146:VAL:HG12  | 1.90                     | 0.53              |
| 3:V:250:ASP:HB2   | 3:V:253:LEU:HD13  | 1.91                     | 0.53              |
| 5:X:516:ASP:N     | 5:X:516:ASP:OD1   | 2.41                     | 0.53              |
| 6:Y:252:LEU:HD11  | 6:Y:262:THR:HG23  | 1.90                     | 0.53              |
| 6:Y:338:PHE:HA    | 6:Y:342:LEU:HD21  | 1.90                     | 0.53              |
| 6:Y:1348:LYS:HA   | 6:Y:1351:VAL:HG22 | 1.90                     | 0.53              |
| 8:L:4:DC:H2'      | 8:L:5:DA:H8       | 1.71                     | 0.53              |
| 1:d:213:PRO:O     | 1:d:217:THR:HG23  | 2.08                     | 0.53              |
| 2:A:104:ARG:NH2   | 5:X:866:ASP:O     | 2.41                     | 0.53              |
| 3:U:45:ARG:HG2    | 5:X:1083:GLU:HB2  | 1.91                     | 0.53              |
| 6:Y:926:PRO:HB3   | 6:Y:1246:VAL:HG11 | 1.91                     | 0.53              |
| 1:c:49:ILE:HB     | 1:c:101:ILE:HG13  | 1.90                     | 0.53              |
| 1:c:86:ILE:HA     | 1:c:91:LEU:HD13   | 1.90                     | 0.53              |
| 1:d:49:ILE:HB     | 1:d:101:ILE:HG13  | 1.90                     | 0.53              |
| 2:A:75:ILE:HG23   | 2:A:79:ALA:HB3    | 1.91                     | 0.53              |
| 5:X:155:VAL:HG12  | 5:X:176:ILE:HG12  | 1.90                     | 0.53              |
| 5:X:213:LEU:HD13  | 5:X:422:LYS:HG2   | 1.90                     | 0.53              |
| 6:Y:18:ASP:OD1    | 6:Y:1373:ARG:NH2  | 2.41                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Y:127:LEU:O     | 6:Y:220:ARG:NH2   | 2.40                     | 0.53              |
| 6:Y:482:ALA:O     | 6:Y:488:ASN:ND2   | 2.42                     | 0.53              |
| 6:Y:1025:MET:HB2  | 6:Y:1124:ILE:HB   | 1.90                     | 0.53              |
| 6:Y:1307:LEU:HD13 | 6:Y:1311:LYS:HB2  | 1.90                     | 0.53              |
| 1:a:369:GLU:HG2   | 1:a:370:LEU:HD12  | 1.91                     | 0.53              |
| 1:b:171:GLY:N     | 1:b:314:THR:OG1   | 2.39                     | 0.53              |
| 6:Y:1060:VAL:HG23 | 6:Y:1106:ILE:HG12 | 1.91                     | 0.53              |
| 1:a:95:ASP:OD1    | 1:a:120:ASN:ND2   | 2.30                     | 0.53              |
| 1:b:369:GLU:HG2   | 1:b:370:LEU:HD12  | 1.91                     | 0.53              |
| 1:d:65:LEU:HB2    | 1:d:79:ILE:HB     | 1.91                     | 0.53              |
| 7:K:-17:DG:H2''   | 7:K:-16:DA:H8     | 1.73                     | 0.53              |
| 1:f:56:GLU:HB2    | 1:f:245:MET:SD    | 2.49                     | 0.53              |
| 1:f:65:LEU:HB2    | 1:f:79:ILE:HB     | 1.91                     | 0.53              |
| 1:a:29:MET:HB3    | 1:a:33:ASP:HB3    | 1.91                     | 0.53              |
| 1:a:65:LEU:HB2    | 1:a:79:ILE:HB     | 1.91                     | 0.53              |
| 1:d:56:GLU:HB2    | 1:d:245:MET:SD    | 2.49                     | 0.53              |
| 2:A:62:TRP:HD1    | 2:A:92:TYR:HA     | 1.74                     | 0.53              |
| 3:U:218:ARG:HH22  | 3:V:234:LEU:HG    | 1.74                     | 0.53              |
| 5:X:66:SER:HB2    | 5:X:104:ILE:HG22  | 1.90                     | 0.53              |
| 6:Y:186:GLN:HB2   | 6:Y:238:ILE:HD13  | 1.91                     | 0.53              |
| 6:Y:640:GLY:N     | 6:Y:643:ASP:OD2   | 2.41                     | 0.53              |
| 6:Y:803:VAL:HG13  | 6:Y:1256:ILE:HD11 | 1.91                     | 0.53              |
| 1:f:49:ILE:HB     | 1:f:101:ILE:HG13  | 1.90                     | 0.53              |
| 1:c:369:GLU:HG2   | 1:c:370:LEU:HD12  | 1.91                     | 0.53              |
| 6:Y:337:ARG:HA    | 6:Y:341:ASN:HD22  | 1.74                     | 0.53              |
| 6:Y:1146:GLU:HB3  | 6:Y:1148:ARG:HG3  | 1.91                     | 0.53              |
| 9:R:91:G:O2'      | 9:R:92:C:O4'      | 2.26                     | 0.53              |
| 1:f:86:ILE:HA     | 1:f:91:LEU:HD13   | 1.90                     | 0.53              |
| 1:a:49:ILE:HB     | 1:a:101:ILE:HG13  | 1.90                     | 0.53              |
| 1:a:394:ASP:OD1   | 1:a:394:ASP:N     | 2.42                     | 0.53              |
| 1:e:369:GLU:HG2   | 1:e:370:LEU:HD12  | 1.91                     | 0.53              |
| 2:A:51:ARG:H      | 2:A:51:ARG:HD3    | 1.74                     | 0.53              |
| 5:X:210:LEU:HD22  | 5:X:220:ILE:HG12  | 1.91                     | 0.53              |
| 1:a:213:PRO:O     | 1:a:217:THR:HG23  | 2.08                     | 0.52              |
| 1:c:65:LEU:HB2    | 1:c:79:ILE:HB     | 1.91                     | 0.52              |
| 1:e:213:PRO:O     | 1:e:217:THR:HG23  | 2.08                     | 0.52              |
| 2:A:236:ILE:HG23  | 2:A:273:ILE:HA    | 1.91                     | 0.52              |
| 1:f:213:PRO:O     | 1:f:217:THR:HG23  | 2.08                     | 0.52              |
| 1:a:72:TYR:HB3    | 1:a:245:MET:HE1   | 1.90                     | 0.52              |
| 1:c:72:TYR:HB3    | 1:c:245:MET:HE1   | 1.90                     | 0.52              |
| 12:c:504:BEF:F2   | 10:d:1000:ADP:O2B | 2.17                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:e:394:ASP:OD1  | 1:e:394:ASP:N     | 2.42                     | 0.52              |
| 2:A:162:ILE:HG12 | 2:A:197:VAL:O     | 2.10                     | 0.52              |
| 5:X:236:LYS:HG2  | 5:X:286:GLU:HG3   | 1.90                     | 0.52              |
| 6:Y:1079:LYS:HD2 | 6:Y:1098:GLN:HB3  | 1.91                     | 0.52              |
| 1:f:369:GLU:HG2  | 1:f:370:LEU:HD12  | 1.91                     | 0.52              |
| 1:b:29:MET:HB3   | 1:b:33:ASP:HB3    | 1.91                     | 0.52              |
| 1:c:88:ARG:HH22  | 5:X:998:LEU:HD22  | 1.73                     | 0.52              |
| 2:A:235:LYS:NZ   | 2:A:289:ALA:O     | 2.43                     | 0.52              |
| 5:X:255:ILE:HB   | 5:X:263:VAL:HB    | 1.92                     | 0.52              |
| 1:f:171:GLY:N    | 1:f:314:THR:OG1   | 2.39                     | 0.52              |
| 1:c:29:MET:HB3   | 1:c:33:ASP:HB3    | 1.91                     | 0.52              |
| 1:d:244:GLU:OE2  | 1:d:274:TYR:OH    | 2.11                     | 0.52              |
| 3:V:81:ILE:HD12  | 3:V:131:CYS:SG    | 2.50                     | 0.52              |
| 4:W:60:ASN:H     | 4:W:63:ILE:HB     | 1.74                     | 0.52              |
| 8:L:-8:DC:H2''   | 8:L:-7:DG:H8      | 1.74                     | 0.52              |
| 1:a:173:ARG:NH2  | 1:b:214:GLU:OE1   | 2.42                     | 0.52              |
| 1:a:212:ARG:NH2  | 12:a:1002:BEF:F1  | 2.33                     | 0.52              |
| 1:b:56:GLU:HB2   | 1:b:245:MET:SD    | 2.49                     | 0.52              |
| 1:c:56:GLU:HB2   | 1:c:245:MET:SD    | 2.49                     | 0.52              |
| 1:c:171:GLY:N    | 1:c:314:THR:OG1   | 2.39                     | 0.52              |
| 5:X:297:VAL:HB   | 5:X:317:LEU:HD21  | 1.91                     | 0.52              |
| 5:X:1254:VAL:O   | 6:Y:99:ARG:NH2    | 2.41                     | 0.52              |
| 6:Y:133:ARG:NH2  | 6:Y:136:GLU:OE1   | 2.43                     | 0.52              |
| 6:Y:1326:GLN:NE2 | 6:Y:1327:GLU:OE1  | 2.43                     | 0.52              |
| 1:a:56:GLU:HB2   | 1:a:245:MET:SD    | 2.49                     | 0.52              |
| 8:L:6:DC:H2'     | 8:L:7:DA:H8       | 1.73                     | 0.52              |
| 1:f:90:ASN:HB3   | 1:a:28:ARG:CD     | 2.38                     | 0.52              |
| 1:b:213:PRO:O    | 1:b:217:THR:HG23  | 2.08                     | 0.52              |
| 5:X:27:LEU:O     | 5:X:528:ARG:NH1   | 2.37                     | 0.52              |
| 1:e:56:GLU:HB2   | 1:e:245:MET:SD    | 2.49                     | 0.52              |
| 4:W:70:GLN:O     | 4:W:73:GLN:HG3    | 2.10                     | 0.52              |
| 2:A:67:GLU:HG3   | 2:A:69:THR:HG22   | 1.91                     | 0.52              |
| 6:Y:1026:PRO:HB2 | 6:Y:1028:ILE:HG23 | 1.92                     | 0.52              |
| 1:d:3:LEU:HD11   | 1:d:39:LEU:HD11   | 1.92                     | 0.52              |
| 1:d:369:GLU:HG2  | 1:d:370:LEU:HD12  | 1.91                     | 0.52              |
| 1:e:29:MET:HB3   | 1:e:33:ASP:HB3    | 1.91                     | 0.52              |
| 1:f:115:LYS:HB3  | 9:R:19:C:C5       | 2.42                     | 0.51              |
| 1:a:130:LYS:O    | 1:b:27:ALA:HB1    | 2.10                     | 0.51              |
| 1:b:3:LEU:HD11   | 1:b:39:LEU:HD11   | 1.92                     | 0.51              |
| 1:b:133:PHE:N    | 1:b:255:GLU:OE2   | 2.43                     | 0.51              |
| 5:X:812:PHE:HA   | 6:Y:505:ASP:OD2   | 2.11                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Y:1194:ARG:NH1  | 6:Y:1211:SER:OG   | 2.43                     | 0.51              |
| 1:e:65:LEU:HB2    | 1:e:79:ILE:HB     | 1.91                     | 0.51              |
| 1:e:95:ASP:OD1    | 1:e:120:ASN:ND2   | 2.30                     | 0.51              |
| 1:e:160:ARG:NH2   | 1:e:408:THR:O     | 2.44                     | 0.51              |
| 3:V:180:VAL:HA    | 3:V:207:THR:HA    | 1.91                     | 0.51              |
| 5:X:726:TYR:HB3   | 5:X:733:VAL:HB    | 1.92                     | 0.51              |
| 1:f:29:MET:HB3    | 1:f:33:ASP:HB3    | 1.91                     | 0.51              |
| 1:f:160:ARG:NH2   | 1:f:408:THR:O     | 2.44                     | 0.51              |
| 1:b:65:LEU:HB2    | 1:b:79:ILE:HB     | 1.91                     | 0.51              |
| 1:c:244:GLU:OE2   | 1:c:274:TYR:OH    | 2.12                     | 0.51              |
| 1:a:133:PHE:N     | 1:a:255:GLU:OE2   | 2.43                     | 0.51              |
| 1:a:160:ARG:NH2   | 1:a:408:THR:O     | 2.44                     | 0.51              |
| 1:d:95:ASP:OD1    | 1:d:120:ASN:ND2   | 2.30                     | 0.51              |
| 3:U:100:LEU:HD23  | 3:U:115:ILE:HD12  | 1.92                     | 0.51              |
| 5:X:781:ASP:OD1   | 5:X:782:VAL:N     | 2.44                     | 0.51              |
| 5:X:1244:HIS:NE2  | 5:X:1266:GLY:O    | 2.29                     | 0.51              |
| 6:Y:393:THR:HG23  | 6:Y:396:ALA:H     | 1.75                     | 0.51              |
| 8:L:6:DC:H2'      | 8:L:7:DA:C8       | 2.45                     | 0.51              |
| 1:b:160:ARG:NH2   | 1:b:408:THR:O     | 2.44                     | 0.51              |
| 1:d:29:MET:HB3    | 1:d:33:ASP:HB3    | 1.91                     | 0.51              |
| 1:d:394:ASP:OD1   | 1:d:394:ASP:N     | 2.42                     | 0.51              |
| 2:A:154:LEU:HB3   | 2:A:158:ALA:HB3   | 1.91                     | 0.51              |
| 5:X:975:ILE:O     | 5:X:979:LEU:HG    | 2.09                     | 0.51              |
| 5:X:1256:GLN:HE21 | 6:Y:99:ARG:HH12   | 1.56                     | 0.51              |
| 5:X:1277:ALA:HA   | 6:Y:921:GLN:HE22  | 1.76                     | 0.51              |
| 1:f:3:LEU:HD11    | 1:f:39:LEU:HD11   | 1.92                     | 0.51              |
| 1:d:160:ARG:NH2   | 1:d:408:THR:O     | 2.44                     | 0.51              |
| 3:V:154:PRO:HG3   | 6:Y:541:LEU:HD13  | 1.92                     | 0.51              |
| 6:Y:20:ILE:HG21   | 6:Y:1320:ILE:HD11 | 1.92                     | 0.51              |
| 1:c:133:PHE:N     | 1:c:255:GLU:OE2   | 2.43                     | 0.51              |
| 1:c:160:ARG:NH2   | 1:c:408:THR:O     | 2.44                     | 0.51              |
| 1:e:3:LEU:HD11    | 1:e:39:LEU:HD11   | 1.92                     | 0.51              |
| 5:X:822:VAL:HG13  | 5:X:827:ARG:HB3   | 1.93                     | 0.51              |
| 5:X:221:LEU:HD23  | 5:X:298:ALA:HB1   | 1.93                     | 0.51              |
| 5:X:300:ASP:OD1   | 5:X:313:ALA:N     | 2.44                     | 0.51              |
| 6:Y:1172:LYS:HD2  | 6:Y:1191:PRO:HA   | 1.93                     | 0.51              |
| 1:d:171:GLY:N     | 1:d:314:THR:OG1   | 2.39                     | 0.51              |
| 2:A:93:VAL:HG13   | 2:A:95:ASP:H      | 1.76                     | 0.51              |
| 2:A:142:VAL:HG23  | 2:A:175:PRO:HA    | 1.93                     | 0.51              |
| 2:A:187:ARG:O     | 2:A:194:GLN:NE2   | 2.42                     | 0.51              |
| 3:V:27:THR:OG1    | 3:V:200:LYS:NZ    | 2.39                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Y:958:ILE:HG13  | 6:Y:1005:LYS:HE2  | 1.92                     | 0.51              |
| 1:b:275:ASN:HA    | 1:b:293:ALA:HB1   | 1.94                     | 0.51              |
| 1:d:88:ARG:HE     | 2:A:87:LEU:HD22   | 1.76                     | 0.51              |
| 2:A:109:THR:O     | 2:A:113:VAL:HG23  | 2.12                     | 0.51              |
| 2:A:119:ARG:O     | 2:A:122:GLU:HG3   | 2.11                     | 0.51              |
| 6:Y:85:CYS:HB3    | 6:Y:89:GLY:H      | 1.76                     | 0.51              |
| 7:K:4:DG:H2''     | 7:K:5:DA:C8       | 2.45                     | 0.51              |
| 1:a:160:ARG:HB2   | 1:a:403:LEU:HD21  | 1.93                     | 0.50              |
| 1:c:160:ARG:HB2   | 1:c:403:LEU:HD21  | 1.93                     | 0.50              |
| 2:A:413:ALA:HA    | 2:A:416:THR:HG22  | 1.93                     | 0.50              |
| 4:W:44:ASP:OD1    | 4:W:45:LYS:N      | 2.44                     | 0.50              |
| 6:Y:850:LYS:HG2   | 6:Y:851:PRO:HD2   | 1.92                     | 0.50              |
| 6:Y:938:GLY:O     | 6:Y:943:ARG:NH1   | 2.44                     | 0.50              |
| 6:Y:1307:LEU:HD11 | 6:Y:1312:ALA:HB2  | 1.93                     | 0.50              |
| 7:K:4:DG:H2''     | 7:K:5:DA:H8       | 1.76                     | 0.50              |
| 1:d:295:HIS:NE2   | 1:e:233:ASP:O     | 2.43                     | 0.50              |
| 2:A:428:ASN:OD1   | 2:A:430:PRO:HD3   | 2.11                     | 0.50              |
| 1:d:160:ARG:HB2   | 1:d:403:LEU:HD21  | 1.93                     | 0.50              |
| 6:Y:285:LEU:HD21  | 8:L:19:DG:OP1     | 2.11                     | 0.50              |
| 1:f:275:ASN:HA    | 1:f:293:ALA:HB1   | 1.93                     | 0.50              |
| 1:c:3:LEU:HD11    | 1:c:39:LEU:HD11   | 1.92                     | 0.50              |
| 1:d:275:ASN:HA    | 1:d:293:ALA:HB1   | 1.94                     | 0.50              |
| 1:e:275:ASN:HA    | 1:e:293:ALA:HB1   | 1.93                     | 0.50              |
| 2:A:22:LYS:O      | 2:A:117:LYS:NZ    | 2.44                     | 0.50              |
| 3:V:182:ARG:HB3   | 6:Y:531:LYS:HB3   | 1.92                     | 0.50              |
| 5:X:225:PHE:HD2   | 5:X:336:LEU:HD13  | 1.76                     | 0.50              |
| 6:Y:372:MET:HE1   | 6:Y:447:ILE:HD11  | 1.94                     | 0.50              |
| 1:f:133:PHE:N     | 1:f:255:GLU:OE2   | 2.43                     | 0.50              |
| 1:a:3:LEU:HD11    | 1:a:39:LEU:HD11   | 1.92                     | 0.50              |
| 6:Y:660:GLU:O     | 6:Y:663:GLU:HG3   | 2.10                     | 0.50              |
| 6:Y:885:VAL:HG11  | 6:Y:1255:VAL:HG12 | 1.93                     | 0.50              |
| 1:a:86:ILE:HG23   | 1:a:91:LEU:HB2    | 1.94                     | 0.50              |
| 10:e:1000:ADP:O2B | 12:e:1002:BEF:F3  | 2.19                     | 0.50              |
| 5:X:876:GLU:HG3   | 5:X:927:THR:HG22  | 1.93                     | 0.50              |
| 6:Y:830:ASP:OD1   | 6:Y:830:ASP:N     | 2.45                     | 0.50              |
| 1:c:86:ILE:HG23   | 1:c:91:LEU:HB2    | 1.94                     | 0.50              |
| 1:e:86:ILE:HG23   | 1:e:91:LEU:HB2    | 1.94                     | 0.50              |
| 2:A:202:PRO:HB3   | 2:A:228:ARG:HG3   | 1.94                     | 0.50              |
| 5:X:14:ASP:HA     | 5:X:1183:ALA:HB3  | 1.93                     | 0.50              |
| 5:X:207:THR:HG21  | 5:X:351:LEU:HG    | 1.94                     | 0.50              |
| 1:f:231:THR:HG23  | 1:f:233:ASP:H     | 1.77                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:227:ALA:HB1   | 2:A:330:GLN:HE21  | 1.76                     | 0.50              |
| 3:V:102:LEU:HD13  | 3:V:115:ILE:HD13  | 1.93                     | 0.50              |
| 5:X:992:LEU:HG    | 5:X:993:PRO:HD3   | 1.94                     | 0.50              |
| 5:X:1006:GLU:HB2  | 5:X:1010:GLN:HE22 | 1.77                     | 0.50              |
| 5:X:1067:ALA:HB2  | 5:X:1073:LYS:HA   | 1.92                     | 0.50              |
| 5:X:1101:LEU:HD13 | 6:Y:504:GLN:HB2   | 1.93                     | 0.50              |
| 6:Y:949:SER:HB3   | 6:Y:1020:TRP:CD1  | 2.47                     | 0.50              |
| 1:a:275:ASN:HA    | 1:a:293:ALA:HB1   | 1.94                     | 0.50              |
| 1:d:86:ILE:HG23   | 1:d:91:LEU:HB2    | 1.94                     | 0.50              |
| 4:W:42:GLU:HG2    | 4:W:52:ARG:HH22   | 1.76                     | 0.50              |
| 5:X:1107:MET:SD   | 6:Y:739:GLN:NE2   | 2.85                     | 0.50              |
| 6:Y:410:ASP:N     | 6:Y:410:ASP:OD1   | 2.44                     | 0.50              |
| 6:Y:1164:SER:OG   | 6:Y:1165:PHE:N    | 2.45                     | 0.50              |
| 7:K:9:DG:H2"      | 7:K:10:DA:C8      | 2.46                     | 0.50              |
| 1:f:86:ILE:HG23   | 1:f:91:LEU:HB2    | 1.94                     | 0.49              |
| 1:f:394:ASP:OD1   | 1:f:394:ASP:N     | 2.42                     | 0.49              |
| 2:A:76:THR:HG23   | 2:A:78:GLU:H      | 1.77                     | 0.49              |
| 3:V:92:VAL:HG22   | 3:V:121:VAL:HG12  | 1.94                     | 0.49              |
| 1:f:73:LEU:HD21   | 1:f:238:ARG:HD2   | 1.95                     | 0.49              |
| 1:a:73:LEU:HD21   | 1:a:238:ARG:HD2   | 1.94                     | 0.49              |
| 1:b:231:THR:HG23  | 1:b:233:ASP:H     | 1.77                     | 0.49              |
| 2:A:60:ARG:N      | 2:A:93:VAL:O      | 2.38                     | 0.49              |
| 4:W:7:GLN:HE22    | 6:Y:615:LYS:H     | 1.59                     | 0.49              |
| 5:X:187:GLU:O     | 5:X:194:LEU:HD12  | 2.12                     | 0.49              |
| 5:X:423:ASP:OD1   | 5:X:423:ASP:N     | 2.44                     | 0.49              |
| 5:X:483:ASP:OD1   | 5:X:483:ASP:N     | 2.46                     | 0.49              |
| 6:Y:256:ASP:OD1   | 6:Y:256:ASP:N     | 2.45                     | 0.49              |
| 8:L:8:DC:H2'      | 8:L:9:DG:C8       | 2.47                     | 0.49              |
| 1:f:160:ARG:HB2   | 1:f:403:LEU:HD21  | 1.93                     | 0.49              |
| 1:c:394:ASP:OD1   | 1:c:394:ASP:N     | 2.42                     | 0.49              |
| 2:A:247:PRO:HG3   | 2:A:275:LEU:HD13  | 1.94                     | 0.49              |
| 5:X:156:PHE:HE1   | 5:X:450:ASN:HB3   | 1.77                     | 0.49              |
| 6:Y:952:VAL:HG11  | 6:Y:984:LEU:HD13  | 1.94                     | 0.49              |
| 1:e:231:THR:HG23  | 1:e:233:ASP:H     | 1.77                     | 0.49              |
| 2:A:97:ILE:HG22   | 2:A:98:GLU:N      | 2.26                     | 0.49              |
| 5:X:804:PHE:HE1   | 5:X:1098:LEU:HD12 | 1.77                     | 0.49              |
| 6:Y:868:TRP:O     | 6:Y:872:LEU:HD23  | 2.13                     | 0.49              |
| 1:b:160:ARG:HB2   | 1:b:403:LEU:HD21  | 1.93                     | 0.49              |
| 10:c:501:ADP:O2B  | 12:c:503:BEF:F2   | 2.20                     | 0.49              |
| 1:d:173:ARG:HH22  | 1:e:214:GLU:CD    | 2.19                     | 0.49              |
| 1:d:349:ILE:HG12  | 1:d:393:ILE:HG12  | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Y:80:HIS:HB3    | 6:Y:83:VAL:HB     | 1.95                     | 0.49              |
| 6:Y:339:ARG:HD3   | 6:Y:343:LEU:HD12  | 1.94                     | 0.49              |
| 7:K:-13:DA:H2''   | 7:K:-12:DG:N7     | 2.27                     | 0.49              |
| 7:K:3:DT:H2''     | 7:K:4:DG:H8       | 1.78                     | 0.49              |
| 9:R:94:U:H2'      | 9:R:95:G:C8       | 2.48                     | 0.49              |
| 1:b:173:ARG:HH21  | 1:c:212:ARG:HB3   | 1.76                     | 0.49              |
| 1:b:384:ARG:HD2   | 1:c:353:ARG:HH22  | 1.78                     | 0.49              |
| 1:e:348:LYS:O     | 1:e:352:LYS:HB2   | 2.13                     | 0.49              |
| 3:V:279:GLY:HA3   | 3:V:321:TRP:CE2   | 2.48                     | 0.49              |
| 5:X:1223:ARG:HH22 | 6:Y:719:PHE:HB2   | 1.78                     | 0.49              |
| 5:X:1335:ILE:O    | 5:X:1335:ILE:HG13 | 2.13                     | 0.49              |
| 6:Y:517:CYS:H     | 6:Y:545:HIS:HD2   | 1.59                     | 0.49              |
| 6:Y:1233:ILE:O    | 6:Y:1237:VAL:HG23 | 2.13                     | 0.49              |
| 1:a:108:GLU:HB3   | 8:L:21:DC:C4      | 2.48                     | 0.49              |
| 1:c:275:ASN:HA    | 1:c:293:ALA:HB1   | 1.93                     | 0.49              |
| 2:A:282:GLN:HA    | 2:A:285:ILE:HD12  | 1.95                     | 0.49              |
| 3:U:174:ASP:OD1   | 3:U:174:ASP:N     | 2.45                     | 0.49              |
| 1:a:182:ALA:HA    | 1:a:350:ALA:HB1   | 1.95                     | 0.49              |
| 1:b:73:LEU:HD21   | 1:b:238:ARG:HD2   | 1.94                     | 0.49              |
| 1:b:394:ASP:N     | 1:b:394:ASP:OD1   | 2.42                     | 0.49              |
| 1:f:384:ARG:HA    | 1:f:387:ILE:HG22  | 1.95                     | 0.49              |
| 1:b:348:LYS:O     | 1:b:352:LYS:HB2   | 2.13                     | 0.49              |
| 1:b:384:ARG:HA    | 1:b:387:ILE:HG22  | 1.95                     | 0.49              |
| 1:c:348:LYS:O     | 1:c:352:LYS:HB2   | 2.13                     | 0.49              |
| 1:d:231:THR:HG23  | 1:d:233:ASP:H     | 1.77                     | 0.49              |
| 3:V:262:LEU:HD23  | 3:V:262:LEU:H     | 1.77                     | 0.49              |
| 3:V:270:LEU:HD21  | 3:V:281:LEU:HD22  | 1.94                     | 0.49              |
| 6:Y:516:ASP:HA    | 6:Y:545:HIS:HB2   | 1.95                     | 0.49              |
| 9:R:20:A:H2'      | 9:R:21:C:C6       | 2.48                     | 0.49              |
| 1:a:231:THR:HG23  | 1:a:233:ASP:H     | 1.77                     | 0.49              |
| 1:a:347:ARG:O     | 1:a:351:GLU:HG2   | 2.13                     | 0.49              |
| 1:c:73:LEU:HD21   | 1:c:238:ARG:HD2   | 1.95                     | 0.49              |
| 6:Y:54:ASP:OD1    | 6:Y:54:ASP:N      | 2.45                     | 0.49              |
| 1:e:160:ARG:HB2   | 1:e:403:LEU:HD21  | 1.93                     | 0.48              |
| 1:e:384:ARG:HA    | 1:e:387:ILE:HG22  | 1.95                     | 0.48              |
| 5:X:952:GLN:HG3   | 5:X:1036:ILE:HD12 | 1.95                     | 0.48              |
| 5:X:1225:VAL:HG23 | 6:Y:638:SER:HB2   | 1.95                     | 0.48              |
| 6:Y:1326:GLN:HG2  | 6:Y:1327:GLU:N    | 2.28                     | 0.48              |
| 1:a:384:ARG:HA    | 1:a:387:ILE:HG22  | 1.95                     | 0.48              |
| 1:b:347:ARG:O     | 1:b:351:GLU:HG2   | 2.13                     | 0.48              |
| 1:c:349:ILE:HG12  | 1:c:393:ILE:HG12  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:e:349:ILE:HG12 | 1:e:393:ILE:HG12  | 1.95                     | 0.48              |
| 5:X:842:ASP:N    | 5:X:1045:GLY:O    | 2.41                     | 0.48              |
| 5:X:972:PHE:O    | 5:X:975:ILE:HG22  | 2.13                     | 0.48              |
| 5:X:1070:HIS:CG  | 5:X:1111:GLN:HB3  | 2.48                     | 0.48              |
| 8:L:-4:DC:C2     | 8:L:-3:DA:N7      | 2.81                     | 0.48              |
| 1:f:348:LYS:O    | 1:f:352:LYS:HB2   | 2.13                     | 0.48              |
| 1:f:349:ILE:HG12 | 1:f:393:ILE:HG12  | 1.95                     | 0.48              |
| 1:b:349:ILE:HG12 | 1:b:393:ILE:HG12  | 1.95                     | 0.48              |
| 1:d:133:PHE:N    | 1:d:255:GLU:OE2   | 2.43                     | 0.48              |
| 1:e:184:LYS:NZ   | 12:e:1002:BEF:F2  | 2.36                     | 0.48              |
| 2:A:80:ALA:HB1   | 2:A:86:SER:H      | 1.77                     | 0.48              |
| 3:V:316:MET:O    | 3:V:317:ARG:NH1   | 2.46                     | 0.48              |
| 5:X:721:GLY:N    | 5:X:740:GLU:OE2   | 2.46                     | 0.48              |
| 5:X:765:ILE:HG13 | 5:X:787:PRO:HG3   | 1.96                     | 0.48              |
| 5:X:946:LEU:O    | 5:X:949:GLU:HG3   | 2.13                     | 0.48              |
| 6:Y:282:LEU:HA   | 6:Y:285:LEU:HB3   | 1.95                     | 0.48              |
| 6:Y:377:PHE:HD1  | 6:Y:380:PHE:HD2   | 1.60                     | 0.48              |
| 6:Y:553:THR:HG22 | 6:Y:567:THR:HG22  | 1.94                     | 0.48              |
| 6:Y:1035:VAL:HB  | 6:Y:1115:ILE:HD13 | 1.95                     | 0.48              |
| 1:f:347:ARG:O    | 1:f:351:GLU:HG2   | 2.13                     | 0.48              |
| 1:c:231:THR:HG23 | 1:c:233:ASP:H     | 1.77                     | 0.48              |
| 1:c:347:ARG:O    | 1:c:351:GLU:HG2   | 2.13                     | 0.48              |
| 1:c:384:ARG:HA   | 1:c:387:ILE:HG22  | 1.95                     | 0.48              |
| 1:d:348:LYS:O    | 1:d:352:LYS:HB2   | 2.13                     | 0.48              |
| 1:e:347:ARG:O    | 1:e:351:GLU:HG2   | 2.13                     | 0.48              |
| 5:X:1062:PRO:HA  | 5:X:1076:ILE:HG23 | 1.94                     | 0.48              |
| 5:X:1209:GLN:HA  | 5:X:1226:THR:HA   | 1.94                     | 0.48              |
| 6:Y:753:SER:OG   | 6:Y:754:ILE:N     | 2.45                     | 0.48              |
| 6:Y:979:ASN:ND2  | 6:Y:1208:ASP:OD2  | 2.47                     | 0.48              |
| 2:A:123:ARG:HD2  | 2:A:194:GLN:HB2   | 1.93                     | 0.48              |
| 6:Y:502:PRO:HG2  | 6:Y:601:ILE:HD13  | 1.96                     | 0.48              |
| 1:a:348:LYS:O    | 1:a:352:LYS:HB2   | 2.13                     | 0.48              |
| 1:b:86:ILE:HG23  | 1:b:91:LEU:HB2    | 1.94                     | 0.48              |
| 3:V:46:ILE:HD11  | 3:V:224:LEU:HD13  | 1.95                     | 0.48              |
| 5:X:12:ARG:HD3   | 5:X:1183:ALA:HB2  | 1.96                     | 0.48              |
| 5:X:198:ILE:O    | 5:X:201:ARG:HG2   | 2.13                     | 0.48              |
| 5:X:398:SER:OG   | 5:X:399:ALA:N     | 2.46                     | 0.48              |
| 1:a:327:MET:O    | 1:a:331:ILE:HG12  | 2.14                     | 0.48              |
| 1:c:182:ALA:HA   | 1:c:350:ALA:HB1   | 1.95                     | 0.48              |
| 1:c:327:MET:O    | 1:c:331:ILE:HG12  | 2.14                     | 0.48              |
| 5:X:701:GLY:N    | 5:X:1182:ILE:O    | 2.42                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:X:1131:MET:SD  | 5:X:1141:LEU:HA   | 2.53                     | 0.48              |
| 6:Y:537:TYR:OH   | 6:Y:634:ARG:NH2   | 2.47                     | 0.48              |
| 9:R:96:U:H2'     | 9:R:97:G:C8       | 2.48                     | 0.48              |
| 1:a:183:GLY:HA3  | 10:a:1000:ADP:H8  | 1.79                     | 0.48              |
| 1:b:327:MET:O    | 1:b:331:ILE:HG12  | 2.14                     | 0.48              |
| 1:d:73:LEU:HD21  | 1:d:238:ARG:HD2   | 1.94                     | 0.48              |
| 1:e:133:PHE:N    | 1:e:255:GLU:OE2   | 2.43                     | 0.48              |
| 4:W:16:ARG:HB3   | 6:Y:483:LEU:HD11  | 1.96                     | 0.48              |
| 6:Y:119:SER:OG   | 6:Y:121:PRO:O     | 2.25                     | 0.48              |
| 6:Y:249:LEU:HD12 | 6:Y:249:LEU:H     | 1.79                     | 0.48              |
| 1:e:394:ASP:O    | 1:e:397:GLU:HG3   | 2.14                     | 0.48              |
| 2:A:9:VAL:HG23   | 2:A:23:ILE:HG21   | 1.96                     | 0.48              |
| 5:X:195:PHE:HA   | 5:X:205:PRO:HA    | 1.95                     | 0.48              |
| 6:Y:115:TRP:HH2  | 6:Y:332:LYS:HZ3   | 1.61                     | 0.48              |
| 6:Y:613:GLY:O    | 6:Y:617:THR:OG1   | 2.32                     | 0.48              |
| 6:Y:705:THR:HG21 | 6:Y:718:SER:HA    | 1.95                     | 0.48              |
| 6:Y:1002:VAL:N   | 6:Y:1019:ASN:O    | 2.42                     | 0.48              |
| 1:a:349:ILE:HG12 | 1:a:393:ILE:HG12  | 1.95                     | 0.48              |
| 1:d:384:ARG:HA   | 1:d:387:ILE:HG22  | 1.95                     | 0.48              |
| 1:e:73:LEU:HD21  | 1:e:238:ARG:HD2   | 1.94                     | 0.48              |
| 2:A:114:ILE:O    | 2:A:118:VAL:HG13  | 2.14                     | 0.48              |
| 2:A:373:LEU:HD11 | 2:A:395:ILE:HG12  | 1.96                     | 0.48              |
| 5:X:735:LYS:HA   | 5:X:748:ILE:HG22  | 1.95                     | 0.48              |
| 5:X:1196:LYS:HD2 | 5:X:1206:THR:HG22 | 1.94                     | 0.48              |
| 1:f:201:ASP:OD1  | 1:f:201:ASP:N     | 2.47                     | 0.47              |
| 1:f:327:MET:O    | 1:f:331:ILE:HG12  | 2.14                     | 0.47              |
| 1:a:171:GLY:N    | 1:a:314:THR:OG1   | 2.39                     | 0.47              |
| 1:a:394:ASP:O    | 1:a:397:GLU:HG3   | 2.14                     | 0.47              |
| 1:b:394:ASP:O    | 1:b:397:GLU:HG3   | 2.14                     | 0.47              |
| 1:d:327:MET:O    | 1:d:331:ILE:HG12  | 2.14                     | 0.47              |
| 1:d:347:ARG:O    | 1:d:351:GLU:HG2   | 2.13                     | 0.47              |
| 3:V:93:GLN:O     | 3:V:148:ARG:NH2   | 2.46                     | 0.47              |
| 3:V:196:THR:OG1  | 3:V:197:ASP:N     | 2.47                     | 0.47              |
| 4:W:9:ALA:HB1    | 4:W:19:LEU:HD11   | 1.95                     | 0.47              |
| 5:X:263:VAL:HG21 | 5:X:269:ILE:HG12  | 1.96                     | 0.47              |
| 5:X:883:LEU:HD11 | 5:X:1052:VAL:HG21 | 1.95                     | 0.47              |
| 6:Y:126:LEU:O    | 6:Y:220:ARG:NH1   | 2.47                     | 0.47              |
| 6:Y:172:PHE:HB2  | 6:Y:176:PHE:HB2   | 1.94                     | 0.47              |
| 6:Y:1161:GLY:HA3 | 6:Y:1179:PRO:HA   | 1.94                     | 0.47              |
| 3:V:112:ALA:HB1  | 3:V:123:ILE:HG21  | 1.95                     | 0.47              |
| 3:V:253:LEU:HA   | 3:V:278:ILE:HB    | 1.96                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:X:889:PRO:HA    | 5:X:912:ASP:HB3  | 1.97                     | 0.47              |
| 6:Y:174:ASP:OD1   | 6:Y:174:ASP:N    | 2.48                     | 0.47              |
| 6:Y:1061:VAL:HG22 | 6:Y:1105:ALA:H   | 1.78                     | 0.47              |
| 1:f:182:ALA:HA    | 1:f:350:ALA:HB1  | 1.95                     | 0.47              |
| 1:f:394:ASP:O     | 1:f:397:GLU:HG3  | 2.14                     | 0.47              |
| 1:b:182:ALA:HA    | 1:b:350:ALA:HB1  | 1.95                     | 0.47              |
| 1:c:115:LYS:HD3   | 5:X:1012:GLU:HB2 | 1.95                     | 0.47              |
| 1:c:372:THR:OG1   | 1:c:376:GLU:HB3  | 2.15                     | 0.47              |
| 5:X:468:LEU:HA    | 5:X:471:VAL:HG12 | 1.96                     | 0.47              |
| 6:Y:58:CYS:SG     | 6:Y:59:ALA:N     | 2.87                     | 0.47              |
| 6:Y:155:GLU:CD    | 6:Y:157:GLN:H    | 2.22                     | 0.47              |
| 6:Y:450:HIS:HB3   | 6:Y:453:VAL:HG12 | 1.97                     | 0.47              |
| 1:c:394:ASP:O     | 1:c:397:GLU:HG3  | 2.14                     | 0.47              |
| 2:A:115:VAL:HA    | 2:A:118:VAL:HG22 | 1.95                     | 0.47              |
| 2:A:400:GLU:HG2   | 2:A:401:PRO:CD   | 2.42                     | 0.47              |
| 3:V:118:ASP:HB2   | 3:V:121:VAL:HG22 | 1.96                     | 0.47              |
| 5:X:130:MET:SD    | 5:X:134:GLY:HA2  | 2.55                     | 0.47              |
| 5:X:800:MET:HE3   | 5:X:800:MET:HB2  | 1.80                     | 0.47              |
| 5:X:1289:GLU:HG3  | 5:X:1294:LYS:HD3 | 1.96                     | 0.47              |
| 6:Y:1050:THR:HG23 | 6:Y:1057:SER:HA  | 1.96                     | 0.47              |
| 1:c:265:ASP:HA    | 1:c:266:SER:HA   | 1.57                     | 0.47              |
| 1:d:182:ALA:HA    | 1:d:350:ALA:HB1  | 1.95                     | 0.47              |
| 2:A:152:LEU:HD11  | 2:A:162:ILE:HD12 | 1.95                     | 0.47              |
| 6:Y:518:VAL:HG23  | 6:Y:547:ARG:HH12 | 1.79                     | 0.47              |
| 1:a:90:ASN:HD22   | 1:a:128:ARG:HB2  | 1.80                     | 0.47              |
| 1:d:236:ALA:HA    | 1:d:239:HIS:HD2  | 1.80                     | 0.47              |
| 3:V:192:VAL:HB    | 3:V:195:ARG:HB2  | 1.96                     | 0.47              |
| 6:Y:146:VAL:HG12  | 6:Y:178:ALA:HB2  | 1.97                     | 0.47              |
| 6:Y:1325:PHE:CG   | 6:Y:1326:GLN:N   | 2.82                     | 0.47              |
| 1:a:147:MET:HE1   | 1:a:195:ILE:HD13 | 1.97                     | 0.47              |
| 1:a:244:GLU:OE2   | 1:a:274:TYR:OH   | 2.12                     | 0.47              |
| 1:a:265:ASP:HA    | 1:a:266:SER:HA   | 1.57                     | 0.47              |
| 1:a:372:THR:OG1   | 1:a:376:GLU:HB3  | 2.15                     | 0.47              |
| 1:b:236:ALA:HA    | 1:b:239:HIS:HD2  | 1.80                     | 0.47              |
| 1:c:195:ILE:HG21  | 1:c:204:LEU:HD13 | 1.97                     | 0.47              |
| 1:c:236:ALA:HA    | 1:c:239:HIS:HD2  | 1.80                     | 0.47              |
| 1:d:394:ASP:O     | 1:d:397:GLU:HG3  | 2.14                     | 0.47              |
| 1:e:90:ASN:HD22   | 1:e:128:ARG:HB2  | 1.80                     | 0.47              |
| 1:e:182:ALA:HA    | 1:e:350:ALA:HB1  | 1.95                     | 0.47              |
| 2:A:127:VAL:O     | 2:A:131:ARG:HB2  | 2.14                     | 0.47              |
| 3:U:64:VAL:HG21   | 3:U:78:ILE:HG13  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:X:812:PHE:HB3   | 6:Y:357:VAL:HG21  | 1.97                     | 0.47              |
| 5:X:1070:HIS:O    | 5:X:1108:ASN:ND2  | 2.39                     | 0.47              |
| 6:Y:71:LEU:H      | 6:Y:90:VAL:HG21   | 1.79                     | 0.47              |
| 6:Y:339:ARG:HA    | 6:Y:343:LEU:HD12  | 1.96                     | 0.47              |
| 8:L:-8:DC:H2'     | 8:L:-7:DG:C8      | 2.49                     | 0.47              |
| 9:R:19:C:H2'      | 9:R:20:A:C8       | 2.49                     | 0.47              |
| 1:f:195:ILE:HG21  | 1:f:204:LEU:HD13  | 1.97                     | 0.47              |
| 1:a:6:LEU:O       | 1:a:9:THR:OG1     | 2.31                     | 0.47              |
| 2:A:122:GLU:O     | 2:A:125:MET:HG3   | 2.15                     | 0.47              |
| 2:A:399:ASP:HB3   | 2:A:401:PRO:HD2   | 1.97                     | 0.47              |
| 3:U:163:GLU:HA    | 3:U:166:ARG:HG3   | 1.95                     | 0.47              |
| 5:X:366:ILE:HG23  | 5:X:370:MET:HE2   | 1.97                     | 0.47              |
| 5:X:658:GLN:HG2   | 5:X:1186:VAL:HG22 | 1.97                     | 0.47              |
| 5:X:1151:LEU:HD11 | 5:X:1197:GLU:HG3  | 1.97                     | 0.47              |
| 6:Y:684:ASP:OD1   | 6:Y:684:ASP:N     | 2.48                     | 0.47              |
| 6:Y:930:LEU:HD12  | 6:Y:1138:LEU:HD13 | 1.97                     | 0.47              |
| 1:f:90:ASN:HD22   | 1:f:128:ARG:HB2   | 1.80                     | 0.47              |
| 1:a:195:ILE:HG21  | 1:a:204:LEU:HD13  | 1.97                     | 0.47              |
| 1:b:90:ASN:HD22   | 1:b:128:ARG:HB2   | 1.80                     | 0.47              |
| 1:b:195:ILE:HG21  | 1:b:204:LEU:HD13  | 1.97                     | 0.47              |
| 1:e:147:MET:HE1   | 1:e:195:ILE:HD13  | 1.97                     | 0.47              |
| 1:e:327:MET:O     | 1:e:331:ILE:HG12  | 2.14                     | 0.47              |
| 2:A:64:VAL:HB     | 2:A:89:LEU:HA     | 1.96                     | 0.47              |
| 2:A:434:LEU:HD11  | 2:A:448:LEU:HD11  | 1.97                     | 0.47              |
| 3:V:111:THR:HG23  | 3:V:113:ALA:H     | 1.80                     | 0.47              |
| 5:X:559:CYS:HB2   | 5:X:662:SER:HB3   | 1.97                     | 0.47              |
| 6:Y:473:THR:HG22  | 6:Y:476:ALA:H     | 1.80                     | 0.47              |
| 6:Y:490:ILE:HA    | 6:Y:500:ILE:HD11  | 1.96                     | 0.47              |
| 6:Y:746:LEU:HD13  | 6:Y:754:ILE:HG21  | 1.97                     | 0.47              |
| 9:R:94:U:H2'      | 9:R:95:G:H8       | 1.80                     | 0.47              |
| 1:b:147:MET:HE1   | 1:b:195:ILE:HD13  | 1.97                     | 0.47              |
| 1:b:372:THR:OG1   | 1:b:376:GLU:HB3   | 2.15                     | 0.47              |
| 1:d:195:ILE:HG21  | 1:d:204:LEU:HD13  | 1.97                     | 0.47              |
| 1:e:184:LYS:N     | 10:e:1000:ADP:O1B | 2.48                     | 0.47              |
| 1:e:195:ILE:HG21  | 1:e:204:LEU:HD13  | 1.97                     | 0.47              |
| 3:V:284:ARG:HH21  | 3:V:288:GLU:HB3   | 1.80                     | 0.47              |
| 5:X:982:GLY:H     | 5:X:1007:LYS:NZ   | 2.12                     | 0.47              |
| 6:Y:452:LEU:HD21  | 6:Y:500:ILE:HA    | 1.96                     | 0.47              |
| 6:Y:740:LEU:HA    | 6:Y:763:PHE:HD2   | 1.80                     | 0.47              |
| 1:d:90:ASN:HD22   | 1:d:128:ARG:HB2   | 1.80                     | 0.46              |
| 5:X:1340:GLU:HG3  | 6:Y:1341:ARG:HE   | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:b:1000:ADP:O1B | 12:b:1002:BEF:F3  | 2.23                     | 0.46              |
| 2:A:24:PHE:CG     | 2:A:51:ARG:HG3    | 2.50                     | 0.46              |
| 5:X:302:ILE:HA    | 5:X:309:LEU:HA    | 1.97                     | 0.46              |
| 6:Y:201:LEU:HD21  | 6:Y:220:ARG:HB3   | 1.97                     | 0.46              |
| 6:Y:503:SER:OG    | 6:Y:504:GLN:N     | 2.46                     | 0.46              |
| 1:f:95:ASP:OD1    | 1:f:120:ASN:ND2   | 2.30                     | 0.46              |
| 3:U:77:ASP:O      | 3:U:81:ILE:HG13   | 2.16                     | 0.46              |
| 5:X:802:VAL:HA    | 5:X:1096:ILE:O    | 2.14                     | 0.46              |
| 5:X:890:LYS:HG2   | 5:X:912:ASP:HA    | 1.98                     | 0.46              |
| 5:X:1102:GLY:HA3  | 5:X:1106:ARG:HH11 | 1.80                     | 0.46              |
| 5:X:1185:PRO:HG2  | 5:X:1188:ASP:HB3  | 1.97                     | 0.46              |
| 5:X:1219:GLU:OE1  | 6:Y:634:ARG:NH1   | 2.49                     | 0.46              |
| 6:Y:1281:GLU:OE1  | 6:Y:1284:ARG:N    | 2.45                     | 0.46              |
| 1:f:372:THR:OG1   | 1:f:376:GLU:HB3   | 2.15                     | 0.46              |
| 1:b:173:ARG:NH2   | 1:c:212:ARG:HB3   | 2.31                     | 0.46              |
| 1:d:372:THR:OG1   | 1:d:376:GLU:HB3   | 2.15                     | 0.46              |
| 2:A:224:LYS:HG2   | 2:A:276:TRP:CD2   | 2.50                     | 0.46              |
| 3:V:196:THR:HB    | 6:Y:443:GLU:HG2   | 1.96                     | 0.46              |
| 5:X:768:MET:O     | 5:X:785:ASP:N     | 2.49                     | 0.46              |
| 6:Y:405:GLU:HG3   | 6:Y:407:VAL:HG12  | 1.97                     | 0.46              |
| 6:Y:885:VAL:HG22  | 6:Y:899:TYR:HA    | 1.96                     | 0.46              |
| 1:a:236:ALA:HA    | 1:a:239:HIS:HD2   | 1.80                     | 0.46              |
| 1:e:372:THR:OG1   | 1:e:376:GLU:HB3   | 2.15                     | 0.46              |
| 2:A:246:ASP:OD1   | 2:A:248:VAL:HG12  | 2.15                     | 0.46              |
| 6:Y:35:PHE:CG     | 6:Y:101:ARG:HD2   | 2.50                     | 0.46              |
| 1:f:261:ILE:HG12  | 1:f:314:THR:HB    | 1.98                     | 0.46              |
| 1:c:90:ASN:HD22   | 1:c:128:ARG:HB2   | 1.80                     | 0.46              |
| 3:U:133:LEU:HD11  | 3:U:140:ILE:HG12  | 1.96                     | 0.46              |
| 3:U:165:GLU:HG2   | 3:U:172:LEU:HD11  | 1.98                     | 0.46              |
| 5:X:10:ARG:NH1    | 5:X:793:GLU:OE1   | 2.45                     | 0.46              |
| 5:X:448:LEU:HD21  | 5:X:587:LEU:HD12  | 1.96                     | 0.46              |
| 6:Y:308:ASP:N     | 6:Y:308:ASP:OD1   | 2.47                     | 0.46              |
| 6:Y:968:ASN:HB2   | 6:Y:972:LYS:HB3   | 1.96                     | 0.46              |
| 5:X:472:GLU:HA    | 5:X:475:VAL:HG12  | 1.98                     | 0.46              |
| 5:X:563:THR:HG22  | 5:X:680:LEU:HD11  | 1.97                     | 0.46              |
| 6:Y:1082:ASP:OD1  | 6:Y:1086:ASN:N    | 2.49                     | 0.46              |
| 1:b:6:LEU:O       | 1:b:9:THR:OG1     | 2.31                     | 0.46              |
| 1:c:147:MET:HE1   | 1:c:195:ILE:HD13  | 1.97                     | 0.46              |
| 1:e:236:ALA:HA    | 1:e:239:HIS:HD2   | 1.80                     | 0.46              |
| 4:W:7:GLN:HE22    | 6:Y:614:LEU:H     | 1.64                     | 0.46              |
| 5:X:1209:GLN:HG2  | 5:X:1226:THR:HB   | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:201:ASP:OD1   | 1:a:201:ASP:N     | 2.47                     | 0.46              |
| 1:e:6:LEU:O       | 1:e:9:THR:OG1     | 2.31                     | 0.46              |
| 5:X:1280:ALA:HB3  | 6:Y:431:ARG:HB3   | 1.97                     | 0.46              |
| 7:K:-16:DA:H2"    | 7:K:-15:DG:H8     | 1.80                     | 0.46              |
| 3:U:31:LEU:HB2    | 3:U:199:ASP:HB3   | 1.97                     | 0.46              |
| 3:U:212:ASP:HB3   | 3:U:215:GLU:HB3   | 1.97                     | 0.46              |
| 3:V:58:GLU:HB3    | 3:V:145:LYS:HB3   | 1.98                     | 0.46              |
| 3:V:323:PRO:HA    | 3:V:324:ALA:HA    | 1.52                     | 0.46              |
| 5:X:210:LEU:HD12  | 5:X:429:MET:HE1   | 1.98                     | 0.46              |
| 5:X:216:THR:N     | 5:X:219:GLN:OE1   | 2.45                     | 0.46              |
| 5:X:805:MET:O     | 5:X:811:ASN:ND2   | 2.46                     | 0.46              |
| 5:X:1186:VAL:HG23 | 5:X:1187:PHE:HD1  | 1.81                     | 0.46              |
| 1:f:70:SER:O      | 1:f:70:SER:OG     | 2.34                     | 0.45              |
| 2:A:202:PRO:O     | 2:A:205:LEU:HB2   | 2.15                     | 0.45              |
| 5:X:519:ASN:ND2   | 5:X:521:LEU:HB3   | 2.31                     | 0.45              |
| 5:X:1260:GLY:O    | 5:X:1264:GLN:NE2  | 2.49                     | 0.45              |
| 6:Y:743:MET:HE2   | 6:Y:745:GLY:HA2   | 1.98                     | 0.45              |
| 6:Y:952:VAL:HG23  | 6:Y:1017:VAL:HG11 | 1.98                     | 0.45              |
| 1:b:201:ASP:OD1   | 1:b:201:ASP:N     | 2.47                     | 0.45              |
| 1:c:115:LYS:NZ    | 5:X:1012:GLU:CD   | 2.74                     | 0.45              |
| 2:A:168:LEU:HD22  | 2:A:230:PRO:HB3   | 1.98                     | 0.45              |
| 3:U:45:ARG:HE     | 3:V:38:THR:HB     | 1.80                     | 0.45              |
| 3:V:295:LEU:HD23  | 3:V:295:LEU:HA    | 1.83                     | 0.45              |
| 5:X:201:ARG:HA    | 5:X:201:ARG:HD2   | 1.71                     | 0.45              |
| 1:b:244:GLU:O     | 1:b:247:ILE:HG22  | 2.17                     | 0.45              |
| 2:A:64:VAL:HG13   | 2:A:75:ILE:O      | 2.17                     | 0.45              |
| 2:A:87:LEU:HB2    | 2:A:91:ASP:OD2    | 2.17                     | 0.45              |
| 5:X:543:ALA:HB3   | 5:X:548:ARG:HH21  | 1.81                     | 0.45              |
| 6:Y:964:LYS:HD3   | 6:Y:964:LYS:HA    | 1.83                     | 0.45              |
| 1:f:147:MET:HE1   | 1:f:195:ILE:HD13  | 1.97                     | 0.45              |
| 1:a:139:LEU:HD21  | 1:b:221:ARG:HH21  | 1.81                     | 0.45              |
| 1:d:261:ILE:HG12  | 1:d:314:THR:HB    | 1.98                     | 0.45              |
| 1:e:397:GLU:HA    | 1:e:400:ILE:HG22  | 1.99                     | 0.45              |
| 5:X:890:LYS:H     | 5:X:912:ASP:HB3   | 1.82                     | 0.45              |
| 5:X:1119:MET:HB2  | 5:X:1228:GLY:HA2  | 1.98                     | 0.45              |
| 6:Y:85:CYS:SG     | 6:Y:86:GLU:N      | 2.90                     | 0.45              |
| 1:c:397:GLU:HA    | 1:c:400:ILE:HG22  | 1.99                     | 0.45              |
| 1:d:210:ASP:HB3   | 1:d:269:ARG:HD3   | 1.98                     | 0.45              |
| 3:U:120:ASP:OD1   | 3:U:120:ASP:N     | 2.50                     | 0.45              |
| 5:X:848:GLU:HG2   | 5:X:888:THR:HG22  | 1.99                     | 0.45              |
| 1:f:210:ASP:HB3   | 1:f:269:ARG:HD3   | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:236:ALA:HA   | 1:f:239:HIS:HD2  | 1.80                     | 0.45              |
| 1:a:261:ILE:HG12 | 1:a:314:THR:HB   | 1.98                     | 0.45              |
| 1:b:210:ASP:HB3  | 1:b:269:ARG:HD3  | 1.99                     | 0.45              |
| 1:c:336:LYS:NZ   | 1:d:323:THR:O    | 2.46                     | 0.45              |
| 1:e:244:GLU:O    | 1:e:247:ILE:HG22 | 2.17                     | 0.45              |
| 2:A:62:TRP:CD1   | 2:A:92:TYR:HA    | 2.51                     | 0.45              |
| 3:V:81:ILE:HG23  | 3:V:131:CYS:SG   | 2.56                     | 0.45              |
| 6:Y:289:ASP:O    | 6:Y:292:VAL:HG22 | 2.17                     | 0.45              |
| 6:Y:430:HIS:HA   | 6:Y:921:GLN:HB3  | 1.98                     | 0.45              |
| 1:a:30:ARG:O     | 1:a:34:ILE:HG12  | 2.17                     | 0.45              |
| 1:a:244:GLU:O    | 1:a:247:ILE:HG22 | 2.17                     | 0.45              |
| 5:X:247:ARG:HH21 | 5:X:274:ILE:HD12 | 1.82                     | 0.45              |
| 5:X:702:THR:H    | 5:X:705:GLU:CD   | 2.24                     | 0.45              |
| 6:Y:288:PRO:HG2  | 6:Y:291:ILE:HD12 | 1.99                     | 0.45              |
| 1:c:210:ASP:HB3  | 1:c:269:ARG:HD3  | 1.98                     | 0.45              |
| 1:d:265:ASP:HA   | 1:d:266:SER:HA   | 1.57                     | 0.45              |
| 1:e:210:ASP:HB3  | 1:e:269:ARG:HD3  | 1.98                     | 0.45              |
| 1:e:261:ILE:HG12 | 1:e:314:THR:HB   | 1.98                     | 0.45              |
| 5:X:674:ASP:OD1  | 5:X:674:ASP:N    | 2.49                     | 0.45              |
| 1:a:210:ASP:HB3  | 1:a:269:ARG:HD3  | 1.99                     | 0.45              |
| 1:b:265:ASP:HA   | 1:b:266:SER:HA   | 1.57                     | 0.45              |
| 1:c:30:ARG:O     | 1:c:34:ILE:HG12  | 2.17                     | 0.45              |
| 4:W:28:ARG:NH1   | 6:Y:475:GLU:OE2  | 2.49                     | 0.45              |
| 1:f:397:GLU:HA   | 1:f:400:ILE:HG22 | 1.99                     | 0.45              |
| 1:d:147:MET:HE1  | 1:d:195:ILE:HD13 | 1.97                     | 0.45              |
| 1:d:160:ARG:NH1  | 1:d:403:LEU:O    | 2.51                     | 0.45              |
| 1:d:244:GLU:O    | 1:d:247:ILE:HG22 | 2.17                     | 0.45              |
| 3:U:91:ARG:HB2   | 3:U:210:THR:HG23 | 1.99                     | 0.45              |
| 3:V:155:ALA:O    | 3:V:159:ILE:HG13 | 2.16                     | 0.45              |
| 5:X:358:ASP:OD1  | 5:X:358:ASP:N    | 2.47                     | 0.45              |
| 5:X:596:ASP:OD1  | 5:X:596:ASP:N    | 2.49                     | 0.45              |
| 5:X:720:ARG:HH21 | 5:X:736:VAL:HG21 | 1.82                     | 0.45              |
| 5:X:797:GLY:N    | 5:X:1231:TYR:OH  | 2.50                     | 0.45              |
| 5:X:1146:GLN:NE2 | 5:X:1150:ASP:OD2 | 2.46                     | 0.45              |
| 6:Y:332:LYS:HE3  | 6:Y:1328:THR:HB  | 1.98                     | 0.45              |
| 1:c:6:LEU:O      | 1:c:9:THR:OG1    | 2.31                     | 0.44              |
| 1:c:261:ILE:HG12 | 1:c:314:THR:HB   | 1.98                     | 0.44              |
| 1:d:30:ARG:O     | 1:d:34:ILE:HG12  | 2.17                     | 0.44              |
| 1:e:40:LYS:HB3   | 1:e:40:LYS:HE2   | 1.83                     | 0.44              |
| 1:e:265:ASP:HA   | 1:e:266:SER:HA   | 1.57                     | 0.44              |
| 6:Y:620:PHE:CZ   | 6:Y:624:ILE:HD11 | 2.51                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:f:160:ARG:NH1   | 1:f:403:LEU:O     | 2.51                     | 0.44              |
| 1:b:261:ILE:HG12  | 1:b:314:THR:HB    | 1.98                     | 0.44              |
| 1:c:70:SER:O      | 1:c:70:SER:OG     | 2.34                     | 0.44              |
| 1:d:91:LEU:O      | 1:e:28:ARG:NH1    | 2.48                     | 0.44              |
| 2:A:45:VAL:HG12   | 2:A:60:ARG:HA     | 1.98                     | 0.44              |
| 2:A:201:LYS:HD3   | 2:A:201:LYS:HA    | 1.77                     | 0.44              |
| 5:X:1030:GLU:HG3  | 5:X:1034:ARG:HE   | 1.82                     | 0.44              |
| 5:X:1073:LYS:HD3  | 6:Y:462:ASP:HB2   | 1.99                     | 0.44              |
| 1:f:30:ARG:O      | 1:f:34:ILE:HG12   | 2.17                     | 0.44              |
| 1:f:244:GLU:O     | 1:f:247:ILE:HG22  | 2.17                     | 0.44              |
| 1:b:30:ARG:O      | 1:b:34:ILE:HG12   | 2.17                     | 0.44              |
| 3:V:17:GLU:HG2    | 3:V:19:VAL:HG13   | 1.99                     | 0.44              |
| 5:X:10:ARG:O      | 5:X:706:ARG:NH2   | 2.49                     | 0.44              |
| 5:X:15:PHE:CD2    | 5:X:1190:ALA:HB2  | 2.53                     | 0.44              |
| 5:X:185:ASP:HB2   | 5:X:197:ARG:HG3   | 1.99                     | 0.44              |
| 5:X:1281:TYR:CE1  | 6:Y:431:ARG:HD2   | 2.52                     | 0.44              |
| 6:Y:57:PHE:CE1    | 6:Y:247:PRO:HB3   | 2.53                     | 0.44              |
| 1:a:160:ARG:NH1   | 1:a:403:LEU:O     | 2.51                     | 0.44              |
| 5:X:519:ASN:HD21  | 5:X:796:LEU:HD23  | 1.83                     | 0.44              |
| 5:X:1246:ARG:HH12 | 5:X:1259:LEU:H    | 1.64                     | 0.44              |
| 6:Y:1251:LYS:O    | 6:Y:1255:VAL:HG13 | 2.17                     | 0.44              |
| 1:a:183:GLY:HA3   | 10:a:1000:ADP:C8  | 2.53                     | 0.44              |
| 1:b:26:LEU:HB3    | 1:b:34:ILE:HD12   | 2.00                     | 0.44              |
| 1:d:397:GLU:HA    | 1:d:400:ILE:HG22  | 1.98                     | 0.44              |
| 1:e:29:MET:HE2    | 1:e:29:MET:HB2    | 1.93                     | 0.44              |
| 1:e:139:LEU:HD23  | 1:e:139:LEU:HA    | 1.91                     | 0.44              |
| 2:A:308:ALA:HA    | 2:A:338:VAL:HG23  | 1.98                     | 0.44              |
| 3:U:192:VAL:HG11  | 3:U:195:ARG:HB3   | 1.99                     | 0.44              |
| 3:V:275:ILE:HG21  | 3:V:281:LEU:HD13  | 1.99                     | 0.44              |
| 5:X:13:LYS:O      | 5:X:1183:ALA:N    | 2.48                     | 0.44              |
| 5:X:67:GLU:HB2    | 5:X:103:VAL:HG23  | 2.00                     | 0.44              |
| 6:Y:245:LEU:HB3   | 6:Y:250:ARG:HE    | 1.83                     | 0.44              |
| 6:Y:1238:GLN:NE2  | 6:Y:1248:ILE:O    | 2.38                     | 0.44              |
| 1:a:26:LEU:HB3    | 1:a:34:ILE:HD12   | 2.00                     | 0.44              |
| 1:b:160:ARG:NH1   | 1:b:403:LEU:O     | 2.51                     | 0.44              |
| 1:c:244:GLU:O     | 1:c:247:ILE:HG22  | 2.17                     | 0.44              |
| 2:A:30:ALA:HB1    | 2:A:110:ALA:HA    | 1.98                     | 0.44              |
| 5:X:150:HIS:CE1   | 5:X:454:ARG:HE    | 2.36                     | 0.44              |
| 6:Y:1334:GLU:OE1  | 6:Y:1340:LYS:NZ   | 2.39                     | 0.44              |
| 8:L:22:DG:H8      | 8:L:22:DG:H5'     | 1.81                     | 0.44              |
| 1:a:397:GLU:HA    | 1:a:400:ILE:HG22  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:c:160:ARG:NH1   | 1:c:403:LEU:O     | 2.51                     | 0.44              |
| 1:e:30:ARG:O      | 1:e:34:ILE:HG12   | 2.17                     | 0.44              |
| 2:A:142:VAL:HA    | 2:A:152:LEU:HA    | 2.00                     | 0.44              |
| 3:U:233:ASP:OD1   | 3:U:233:ASP:N     | 2.51                     | 0.44              |
| 5:X:10:ARG:HH22   | 5:X:791:LEU:HB2   | 1.82                     | 0.44              |
| 5:X:1107:MET:HE3  | 5:X:1107:MET:HB2  | 1.91                     | 0.44              |
| 6:Y:907:HIS:ND1   | 6:Y:908:ILE:O     | 2.43                     | 0.44              |
| 5:X:617:ALA:HB3   | 5:X:653:MET:HG3   | 1.99                     | 0.44              |
| 5:X:1077:SER:OG   | 5:X:1078:LYS:N    | 2.50                     | 0.44              |
| 5:X:1088:ASP:OD1  | 5:X:1092:THR:N    | 2.46                     | 0.44              |
| 5:X:1241:ASP:OD1  | 5:X:1241:ASP:N    | 2.45                     | 0.44              |
| 6:Y:741:ALA:O     | 6:Y:762:ASN:ND2   | 2.36                     | 0.44              |
| 6:Y:814:CYS:SG    | 6:Y:816:THR:OG1   | 2.63                     | 0.44              |
| 2:A:35:THR:HA     | 2:A:38:LYS:HE2    | 1.99                     | 0.44              |
| 3:V:37:HIS:CE1    | 5:X:1216:ARG:HD2  | 2.52                     | 0.44              |
| 5:X:444:ASP:OD1   | 5:X:444:ASP:N     | 2.51                     | 0.44              |
| 5:X:1066:MET:HE3  | 5:X:1076:ILE:HB   | 1.98                     | 0.44              |
| 6:Y:220:ARG:HD2   | 6:Y:223:LEU:HD23  | 2.00                     | 0.44              |
| 6:Y:268:LEU:HD11  | 6:Y:324:LEU:HD11  | 2.00                     | 0.44              |
| 6:Y:492:SER:OG    | 6:Y:495:ASN:O     | 2.28                     | 0.44              |
| 6:Y:870:ASP:O     | 6:Y:873:GLU:HG3   | 2.18                     | 0.44              |
| 7:K:-15:DG:H2''   | 7:K:-14:DC:H5     | 1.83                     | 0.44              |
| 1:b:397:GLU:HA    | 1:b:400:ILE:HG22  | 1.99                     | 0.43              |
| 1:d:26:LEU:HB3    | 1:d:34:ILE:HD12   | 2.00                     | 0.43              |
| 5:X:1326:LEU:O    | 5:X:1330:ILE:HG12 | 2.18                     | 0.43              |
| 6:Y:210:SER:OG    | 6:Y:213:LYS:HB3   | 2.17                     | 0.43              |
| 1:b:244:GLU:OE2   | 1:b:274:TYR:OH    | 2.12                     | 0.43              |
| 1:c:26:LEU:HB3    | 1:c:34:ILE:HD12   | 2.00                     | 0.43              |
| 1:c:92:ARG:NH1    | 1:c:255:GLU:OE2   | 2.52                     | 0.43              |
| 2:A:318:ILE:HG22  | 2:A:322:GLY:HA2   | 1.99                     | 0.43              |
| 5:X:1259:LEU:HD23 | 5:X:1264:GLN:HG3  | 1.99                     | 0.43              |
| 6:Y:1262:ARG:NH2  | 6:Y:1315:ALA:O    | 2.51                     | 0.43              |
| 1:a:70:SER:O      | 1:a:70:SER:OG     | 2.34                     | 0.43              |
| 1:a:173:ARG:HH22  | 1:b:214:GLU:CD    | 2.26                     | 0.43              |
| 1:b:189:GLN:NE2   | 1:b:218:GLU:OE2   | 2.52                     | 0.43              |
| 1:d:92:ARG:NH1    | 1:d:255:GLU:OE2   | 2.51                     | 0.43              |
| 1:e:160:ARG:NH1   | 1:e:403:LEU:O     | 2.51                     | 0.43              |
| 1:e:189:GLN:NE2   | 1:e:218:GLU:OE2   | 2.52                     | 0.43              |
| 2:A:46:ARG:HD3    | 2:A:61:ARG:HH21   | 1.84                     | 0.43              |
| 3:U:82:LEU:HD23   | 3:U:85:LEU:HD21   | 1.99                     | 0.43              |
| 3:U:111:THR:HG23  | 3:U:113:ALA:H     | 1.83                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:X:1105:SER:OG  | 5:X:1106:ARG:N    | 2.50                     | 0.43              |
| 1:a:91:LEU:O     | 1:b:28:ARG:NH1    | 2.51                     | 0.43              |
| 1:c:189:GLN:NE2  | 1:c:218:GLU:OE2   | 2.52                     | 0.43              |
| 2:A:274:VAL:HG21 | 2:A:286:ASN:HB3   | 2.00                     | 0.43              |
| 3:U:196:THR:O    | 3:U:198:LEU:HD12  | 2.19                     | 0.43              |
| 6:Y:587:LEU:HD21 | 6:Y:608:CYS:HB2   | 2.01                     | 0.43              |
| 6:Y:808:VAL:HG12 | 6:Y:914:ALA:HB2   | 2.00                     | 0.43              |
| 1:f:97:ILE:HD12  | 1:f:119:VAL:HG22  | 2.01                     | 0.43              |
| 5:X:1276:TRP:HA  | 5:X:1279:GLU:OE2  | 2.18                     | 0.43              |
| 5:X:1279:GLU:HB2 | 6:Y:917:VAL:HG11  | 2.00                     | 0.43              |
| 1:b:92:ARG:NH1   | 1:b:255:GLU:OE2   | 2.52                     | 0.43              |
| 1:b:326:LYS:O    | 1:b:330:VAL:HG13  | 2.19                     | 0.43              |
| 1:d:326:LYS:O    | 1:d:330:VAL:HG13  | 2.19                     | 0.43              |
| 1:e:97:ILE:HD12  | 1:e:119:VAL:HG22  | 2.01                     | 0.43              |
| 3:U:45:ARG:NH1   | 5:X:1084:ASP:OD1  | 2.42                     | 0.43              |
| 5:X:149:LEU:HD11 | 5:X:451:ARG:HB3   | 2.00                     | 0.43              |
| 9:R:93:G:H2'     | 9:R:94:U:C6       | 2.54                     | 0.43              |
| 1:a:92:ARG:NH1   | 1:a:255:GLU:OE2   | 2.52                     | 0.43              |
| 1:c:381:TRP:CD1  | 1:d:353:ARG:HH12  | 2.37                     | 0.43              |
| 1:e:92:ARG:NH1   | 1:e:255:GLU:OE2   | 2.51                     | 0.43              |
| 3:V:32:GLU:HG3   | 3:V:33:ARG:H      | 1.84                     | 0.43              |
| 4:W:56:GLU:HB3   | 4:W:58:LEU:HD22   | 2.00                     | 0.43              |
| 5:X:501:ALA:O    | 5:X:504:GLU:HG3   | 2.19                     | 0.43              |
| 5:X:685:MET:SD   | 5:X:1073:LYS:HB3  | 2.58                     | 0.43              |
| 5:X:984:VAL:O    | 5:X:988:LYS:HG2   | 2.18                     | 0.43              |
| 6:Y:57:PHE:CZ    | 6:Y:252:LEU:HD23  | 2.54                     | 0.43              |
| 6:Y:436:ALA:HB3  | 6:Y:485:MET:HA    | 1.99                     | 0.43              |
| 6:Y:1343:GLU:C   | 6:Y:1344:LEU:HD23 | 2.44                     | 0.43              |
| 1:f:92:ARG:NH1   | 1:f:255:GLU:OE2   | 2.52                     | 0.43              |
| 1:f:265:ASP:HA   | 1:f:266:SER:HA    | 1.57                     | 0.43              |
| 1:f:366:ARG:HG3  | 1:a:181:LYS:NZ    | 2.33                     | 0.43              |
| 1:b:412:PHE:HA   | 1:b:415:MET:SD    | 2.59                     | 0.43              |
| 1:e:26:LEU:HD23  | 1:e:34:ILE:HD12   | 2.01                     | 0.43              |
| 1:e:412:PHE:HA   | 1:e:415:MET:SD    | 2.59                     | 0.43              |
| 2:A:149:ASN:OD1  | 2:A:150:ILE:N     | 2.51                     | 0.43              |
| 5:X:81:ASP:O     | 5:X:85:CYS:N      | 2.46                     | 0.43              |
| 6:Y:40:LYS:HB2   | 6:Y:55:GLY:HA2    | 2.00                     | 0.43              |
| 8:L:-12:DT:H2''  | 8:L:-11:DA:N7     | 2.33                     | 0.43              |
| 1:f:26:LEU:HB3   | 1:f:34:ILE:HD12   | 2.00                     | 0.43              |
| 1:f:247:ILE:HB   | 1:f:300:PHE:CE2   | 2.54                     | 0.43              |
| 1:f:248:GLU:O    | 1:f:252:ARG:HG2   | 2.19                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:f:326:LYS:O     | 1:f:330:VAL:HG13 | 2.19                     | 0.43              |
| 1:a:412:PHE:HA    | 1:a:415:MET:SD   | 2.59                     | 0.43              |
| 1:b:97:ILE:HD12   | 1:b:119:VAL:HG22 | 2.01                     | 0.43              |
| 1:c:248:GLU:O     | 1:c:252:ARG:HG2  | 2.19                     | 0.43              |
| 5:X:79:VAL:HG23   | 5:X:80:PHE:HD2   | 1.83                     | 0.43              |
| 1:c:40:LYS:HE2    | 1:c:40:LYS:HB3   | 1.83                     | 0.43              |
| 1:e:26:LEU:HB3    | 1:e:34:ILE:HD12  | 2.00                     | 0.43              |
| 2:A:344:LEU:HD23  | 2:A:350:ALA:HB3  | 2.01                     | 0.43              |
| 3:V:193:GLU:HB2   | 6:Y:406:ALA:HB1  | 2.01                     | 0.43              |
| 5:X:673:HIS:O     | 5:X:1110:GLY:N   | 2.50                     | 0.43              |
| 5:X:1280:ALA:HB1  | 6:Y:918:ILE:HG22 | 2.00                     | 0.43              |
| 5:X:1325:VAL:HG13 | 6:Y:249:LEU:HD23 | 2.00                     | 0.43              |
| 6:Y:245:LEU:HG    | 6:Y:249:LEU:HD13 | 2.00                     | 0.43              |
| 6:Y:278:ARG:HE    | 6:Y:281:ARG:HH21 | 1.66                     | 0.43              |
| 6:Y:419:HIS:CE1   | 6:Y:471:PRO:HD2  | 2.54                     | 0.43              |
| 6:Y:999:TYR:HD1   | 6:Y:1026:PRO:HG2 | 1.84                     | 0.43              |
| 6:Y:1089:LEU:HD23 | 6:Y:1089:LEU:H   | 1.84                     | 0.43              |
| 1:a:189:GLN:NE2   | 1:a:218:GLU:OE2  | 2.52                     | 0.42              |
| 1:c:412:PHE:HA    | 1:c:415:MET:SD   | 2.59                     | 0.42              |
| 1:d:248:GLU:O     | 1:d:252:ARG:HG2  | 2.19                     | 0.42              |
| 2:A:76:THR:HG22   | 2:A:79:ALA:HB2   | 2.01                     | 0.42              |
| 3:V:249:PHE:HE2   | 3:V:254:LEU:HD11 | 1.84                     | 0.42              |
| 5:X:158:ASP:HB3   | 5:X:173:ASN:HD21 | 1.84                     | 0.42              |
| 5:X:1192:GLU:O    | 5:X:1196:LYS:HG2 | 2.19                     | 0.42              |
| 6:Y:998:PRO:HD3   | 6:Y:1020:TRP:CE2 | 2.54                     | 0.42              |
| 6:Y:1219:ASP:HA   | 6:Y:1222:ARG:HG2 | 2.01                     | 0.42              |
| 1:f:26:LEU:HD23   | 1:f:34:ILE:HD12  | 2.01                     | 0.42              |
| 1:c:272:ARG:HG2   | 1:c:327:MET:SD   | 2.59                     | 0.42              |
| 1:d:272:ARG:HG2   | 1:d:327:MET:SD   | 2.59                     | 0.42              |
| 1:e:326:LYS:O     | 1:e:330:VAL:HG13 | 2.19                     | 0.42              |
| 3:V:5:VAL:HG23    | 3:V:7:GLU:H      | 1.84                     | 0.42              |
| 5:X:200:ARG:HG3   | 7:K:-1:DC:H2"    | 2.01                     | 0.42              |
| 5:X:1313:HIS:HB3  | 6:Y:474:LEU:HB2  | 2.01                     | 0.42              |
| 6:Y:334:LYS:HA    | 6:Y:339:ARG:HG2  | 2.01                     | 0.42              |
| 1:b:40:LYS:HE2    | 1:b:40:LYS:HB3   | 1.83                     | 0.42              |
| 1:b:247:ILE:HB    | 1:b:300:PHE:CE2  | 2.54                     | 0.42              |
| 2:A:238:VAL:O     | 2:A:276:TRP:N    | 2.47                     | 0.42              |
| 5:X:257:ALA:HB2   | 5:X:285:ILE:HG22 | 2.02                     | 0.42              |
| 5:X:322:LEU:HD23  | 5:X:325:LEU:HD21 | 2.00                     | 0.42              |
| 5:X:739:ASP:OD1   | 5:X:740:GLU:N    | 2.53                     | 0.42              |
| 5:X:758:ARG:HD2   | 5:X:835:GLU:HB2  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:X:1101:LEU:HD12 | 6:Y:505:ASP:OD1   | 2.19                     | 0.42              |
| 5:X:1223:ARG:HH21 | 6:Y:512:TYR:HE1   | 1.66                     | 0.42              |
| 6:Y:532:GLU:OE1   | 6:Y:532:GLU:N     | 2.43                     | 0.42              |
| 1:d:97:ILE:HD12   | 1:d:119:VAL:HG22  | 2.00                     | 0.42              |
| 1:d:189:GLN:NE2   | 1:d:218:GLU:OE2   | 2.52                     | 0.42              |
| 1:d:412:PHE:HA    | 1:d:415:MET:SD    | 2.59                     | 0.42              |
| 2:A:71:PRO:HG3    | 3:V:308:ALA:HB3   | 2.01                     | 0.42              |
| 2:A:400:GLU:HA    | 2:A:403:VAL:HG12  | 2.02                     | 0.42              |
| 3:U:179:PRO:C     | 3:U:207:THR:HG1   | 2.23                     | 0.42              |
| 3:U:228:LEU:HD13  | 3:V:224:LEU:HD23  | 2.01                     | 0.42              |
| 5:X:767:GLN:HA    | 5:X:786:GLY:HA2   | 2.01                     | 0.42              |
| 6:Y:844:THR:HA    | 6:Y:882:VAL:HG23  | 2.01                     | 0.42              |
| 6:Y:951:GLN:HG3   | 6:Y:1016:THR:HA   | 2.00                     | 0.42              |
| 1:f:85:GLN:HG2    | 9:R:20:A:H61      | 1.83                     | 0.42              |
| 1:e:183:GLY:H     | 10:e:1000:ADP:PB  | 2.43                     | 0.42              |
| 1:e:247:ILE:HB    | 1:e:300:PHE:CE2   | 2.54                     | 0.42              |
| 3:V:111:THR:OG1   | 3:V:112:ALA:N     | 2.52                     | 0.42              |
| 5:X:459:MET:SD    | 5:X:511:LEU:HD11  | 2.60                     | 0.42              |
| 5:X:594:VAL:HG22  | 5:X:599:VAL:HG13  | 2.01                     | 0.42              |
| 6:Y:934:THR:HG23  | 6:Y:936:HIS:H     | 1.83                     | 0.42              |
| 6:Y:1256:ILE:O    | 6:Y:1260:MET:HG2  | 2.19                     | 0.42              |
| 1:b:248:GLU:O     | 1:b:252:ARG:HG2   | 2.19                     | 0.42              |
| 1:d:247:ILE:HB    | 1:d:300:PHE:CE2   | 2.54                     | 0.42              |
| 2:A:5:ILE:HD13    | 2:A:49:ILE:HG21   | 2.00                     | 0.42              |
| 2:A:150:ILE:CG1   | 2:A:162:ILE:HB    | 2.50                     | 0.42              |
| 5:X:241:LEU:HD12  | 5:X:285:ILE:HD13  | 2.02                     | 0.42              |
| 5:X:582:ASN:N     | 5:X:586:PHE:O     | 2.46                     | 0.42              |
| 5:X:1287:LEU:HD22 | 6:Y:1357:ILE:HD11 | 2.01                     | 0.42              |
| 6:Y:998:PRO:HG2   | 6:Y:1001:ALA:HB2  | 2.01                     | 0.42              |
| 7:K:3:DT:H2"      | 7:K:4:DG:C8       | 2.54                     | 0.42              |
| 1:f:276:THR:O     | 1:f:276:THR:OG1   | 2.38                     | 0.42              |
| 1:f:412:PHE:O     | 1:f:415:MET:HG2   | 2.20                     | 0.42              |
| 1:a:248:GLU:O     | 1:a:252:ARG:HG2   | 2.19                     | 0.42              |
| 1:c:201:ASP:OD1   | 1:c:201:ASP:N     | 2.47                     | 0.42              |
| 1:c:247:ILE:HB    | 1:c:300:PHE:CE2   | 2.54                     | 0.42              |
| 1:e:164:LEU:HD12  | 1:e:164:LEU:HA    | 1.91                     | 0.42              |
| 1:e:276:THR:O     | 1:e:276:THR:OG1   | 2.38                     | 0.42              |
| 2:A:151:SER:C     | 2:A:152:LEU:HD12  | 2.44                     | 0.42              |
| 3:V:220:ALA:O     | 3:V:223:ILE:HG22  | 2.19                     | 0.42              |
| 5:X:35:PHE:CD2    | 5:X:130:MET:HG2   | 2.55                     | 0.42              |
| 6:Y:113:HIS:HB3   | 6:Y:116:PHE:HD2   | 1.83                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:K:9:DG:H2"     | 7:K:10:DA:N7      | 2.35                     | 0.42              |
| 1:f:412:PHE:HA   | 1:f:415:MET:SD    | 2.59                     | 0.42              |
| 1:a:97:ILE:HD12  | 1:a:119:VAL:HG22  | 2.01                     | 0.42              |
| 1:a:272:ARG:HG2  | 1:a:327:MET:SD    | 2.59                     | 0.42              |
| 1:a:326:LYS:O    | 1:a:330:VAL:HG13  | 2.19                     | 0.42              |
| 1:b:73:LEU:HD23  | 1:b:73:LEU:HA     | 1.96                     | 0.42              |
| 1:b:353:ARG:HA   | 1:b:353:ARG:HD3   | 1.94                     | 0.42              |
| 1:c:97:ILE:HD12  | 1:c:119:VAL:HG22  | 2.00                     | 0.42              |
| 2:A:16:LYS:C     | 2:A:16:LYS:HD3    | 2.45                     | 0.42              |
| 2:A:115:VAL:HG12 | 5:X:906:PHE:HE1   | 1.84                     | 0.42              |
| 3:V:77:ASP:O     | 3:V:81:ILE:HG12   | 2.20                     | 0.42              |
| 4:W:45:LYS:O     | 4:W:49:ILE:HG12   | 2.20                     | 0.42              |
| 5:X:816:ILE:O    | 5:X:1076:ILE:HD12 | 2.19                     | 0.42              |
| 6:Y:554:GLU:HG3  | 6:Y:566:LYS:HG3   | 2.01                     | 0.42              |
| 6:Y:1346:GLY:O   | 6:Y:1350:ASN:ND2  | 2.52                     | 0.42              |
| 1:f:272:ARG:HG2  | 1:f:327:MET:SD    | 2.59                     | 0.42              |
| 1:a:26:LEU:HD23  | 1:a:34:ILE:HD12   | 2.01                     | 0.42              |
| 1:a:247:ILE:HB   | 1:a:300:PHE:CE2   | 2.54                     | 0.42              |
| 1:c:26:LEU:HD23  | 1:c:34:ILE:HD12   | 2.01                     | 0.42              |
| 3:V:48:LEU:HD22  | 6:Y:535:ARG:HG3   | 2.02                     | 0.42              |
| 3:V:82:LEU:HB3   | 3:V:173:VAL:HG12  | 2.01                     | 0.42              |
| 6:Y:278:ARG:HG3  | 6:Y:282:LEU:HD23  | 2.02                     | 0.42              |
| 1:b:26:LEU:HD23  | 1:b:34:ILE:HD12   | 2.01                     | 0.42              |
| 1:b:385:LYS:NZ   | 1:c:353:ARG:HB2   | 2.35                     | 0.42              |
| 1:e:201:ASP:OD1  | 1:e:201:ASP:N     | 2.47                     | 0.42              |
| 2:A:61:ARG:HG2   | 2:A:63:LEU:HG     | 2.02                     | 0.42              |
| 5:X:146:VAL:HG13 | 5:X:529:ARG:HB3   | 2.01                     | 0.42              |
| 5:X:198:ILE:HG22 | 5:X:199:ASP:OD1   | 2.19                     | 0.42              |
| 5:X:983:GLY:O    | 5:X:986:ALA:N     | 2.52                     | 0.42              |
| 5:X:1101:LEU:O   | 5:X:1104:PRO:HD2  | 2.20                     | 0.42              |
| 1:a:164:LEU:HD12 | 1:a:164:LEU:HA    | 1.91                     | 0.41              |
| 1:b:272:ARG:HG2  | 1:b:327:MET:SD    | 2.59                     | 0.41              |
| 1:e:248:GLU:O    | 1:e:252:ARG:HG2   | 2.19                     | 0.41              |
| 3:V:190:ALA:HB2  | 3:V:200:LYS:HB2   | 2.02                     | 0.41              |
| 5:X:207:THR:HG23 | 5:X:350:THR:HG22  | 2.02                     | 0.41              |
| 5:X:948:ILE:HG13 | 5:X:949:GLU:N     | 2.35                     | 0.41              |
| 5:X:972:PHE:CE2  | 5:X:995:ASP:HA    | 2.54                     | 0.41              |
| 6:Y:513:MET:HE2  | 6:Y:631:TYR:CG    | 2.54                     | 0.41              |
| 6:Y:573:THR:HG23 | 6:Y:576:ARG:H     | 1.85                     | 0.41              |
| 1:d:290:ASP:HB3  | 1:d:293:ALA:HB2   | 2.02                     | 0.41              |
| 3:U:111:THR:OG1  | 3:U:128:HIS:O     | 2.38                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:V:71:LYS:HE3   | 3:V:140:ILE:HD13  | 2.02                     | 0.41              |
| 3:V:307:LEU:HD23 | 3:V:312:LEU:HD11  | 2.01                     | 0.41              |
| 3:V:321:TRP:HA   | 3:V:322:PRO:HA    | 1.76                     | 0.41              |
| 5:X:221:LEU:HG   | 5:X:336:LEU:HD11  | 2.03                     | 0.41              |
| 5:X:1277:ALA:HB3 | 6:Y:434:ILE:HD12  | 2.02                     | 0.41              |
| 6:Y:499:ILE:HD12 | 6:Y:499:ILE:HA    | 1.93                     | 0.41              |
| 6:Y:674:THR:H    | 6:Y:677:GLU:CD    | 2.28                     | 0.41              |
| 6:Y:937:ILE:HG23 | 6:Y:939:GLY:H     | 1.85                     | 0.41              |
| 6:Y:1322:ALA:HB1 | 6:Y:1331:VAL:HG11 | 2.01                     | 0.41              |
| 6:Y:1358:PRO:HB3 | 6:Y:1366:HIS:CG   | 2.55                     | 0.41              |
| 1:e:70:SER:O     | 1:e:70:SER:OG     | 2.34                     | 0.41              |
| 1:e:412:PHE:O    | 1:e:415:MET:HG2   | 2.20                     | 0.41              |
| 3:V:115:ILE:HG21 | 3:V:123:ILE:HD11  | 2.02                     | 0.41              |
| 5:X:178:PRO:HA   | 5:X:397:LEU:HD12  | 2.03                     | 0.41              |
| 6:Y:926:PRO:HB2  | 6:Y:1241:TYR:HE1  | 1.84                     | 0.41              |
| 6:Y:1326:GLN:HG3 | 8:L:-1:DA:H5'     | 2.02                     | 0.41              |
| 1:f:164:LEU:O    | 1:f:360:TYR:OH    | 2.31                     | 0.41              |
| 1:a:40:LYS:HB3   | 1:a:40:LYS:HE2    | 1.83                     | 0.41              |
| 1:c:276:THR:O    | 1:c:276:THR:OG1   | 2.38                     | 0.41              |
| 1:c:290:ASP:HB3  | 1:c:293:ALA:HB2   | 2.02                     | 0.41              |
| 1:c:326:LYS:O    | 1:c:330:VAL:HG13  | 2.19                     | 0.41              |
| 1:c:412:PHE:O    | 1:c:415:MET:HG2   | 2.20                     | 0.41              |
| 1:d:26:LEU:HD23  | 1:d:34:ILE:HD12   | 2.01                     | 0.41              |
| 2:A:325:VAL:O    | 2:A:329:SER:N     | 2.39                     | 0.41              |
| 3:U:113:ALA:HB2  | 3:U:126:PRO:HB2   | 2.02                     | 0.41              |
| 5:X:152:SER:HB2  | 5:X:452:ARG:HB2   | 2.01                     | 0.41              |
| 5:X:1271:GLY:O   | 5:X:1275:VAL:HG23 | 2.21                     | 0.41              |
| 5:X:1340:GLU:HG3 | 6:Y:1341:ARG:HH21 | 1.85                     | 0.41              |
| 6:Y:587:LEU:HD11 | 6:Y:608:CYS:SG    | 2.61                     | 0.41              |
| 6:Y:1250:ASP:OD1 | 6:Y:1250:ASP:N    | 2.53                     | 0.41              |
| 1:a:412:PHE:O    | 1:a:415:MET:HG2   | 2.20                     | 0.41              |
| 1:b:412:PHE:O    | 1:b:415:MET:HG2   | 2.20                     | 0.41              |
| 1:e:272:ARG:HG2  | 1:e:327:MET:SD    | 2.59                     | 0.41              |
| 2:A:57:ASP:OD1   | 2:A:57:ASP:N      | 2.54                     | 0.41              |
| 5:X:19:PRO:HA    | 5:X:1156:ARG:HD2  | 2.03                     | 0.41              |
| 6:Y:412:LEU:HA   | 6:Y:415:VAL:HG22  | 2.02                     | 0.41              |
| 6:Y:804:ALA:O    | 6:Y:805:GLN:HG3   | 2.20                     | 0.41              |
| 1:b:290:ASP:HB3  | 1:b:293:ALA:HB2   | 2.02                     | 0.41              |
| 1:c:381:TRP:CD1  | 1:d:353:ARG:NH1   | 2.89                     | 0.41              |
| 1:e:290:ASP:HB3  | 1:e:293:ALA:HB2   | 2.02                     | 0.41              |
| 2:A:64:VAL:HG11  | 2:A:88:ASN:O      | 2.20                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:X:349:GLU:HA    | 5:X:352:ARG:HG2  | 2.01                     | 0.41              |
| 5:X:1286:THR:HG23 | 6:Y:476:ALA:HB1  | 2.02                     | 0.41              |
| 6:Y:154:LEU:HD12  | 6:Y:176:PHE:HE1  | 1.86                     | 0.41              |
| 6:Y:555:TYR:HB2   | 6:Y:585:LYS:O    | 2.20                     | 0.41              |
| 7:K:1:DT:C2       | 7:K:2:DG:C8      | 3.09                     | 0.41              |
| 1:f:290:ASP:HB3   | 1:f:293:ALA:HB2  | 2.02                     | 0.41              |
| 2:A:203:GLU:O     | 2:A:206:ILE:HB   | 2.20                     | 0.41              |
| 2:A:209:PHE:HA    | 2:A:212:GLU:HG2  | 2.02                     | 0.41              |
| 5:X:143:ARG:HA    | 5:X:514:PHE:HA   | 2.02                     | 0.41              |
| 5:X:149:LEU:N     | 5:X:531:SER:O    | 2.53                     | 0.41              |
| 5:X:826:ASP:OD1   | 5:X:829:THR:OG1  | 2.25                     | 0.41              |
| 5:X:949:GLU:HA    | 5:X:952:GLN:HG2  | 2.02                     | 0.41              |
| 5:X:1290:MET:HE2  | 5:X:1290:MET:HB2 | 2.01                     | 0.41              |
| 6:Y:85:CYS:H      | 6:Y:90:VAL:H     | 1.68                     | 0.41              |
| 6:Y:161:THR:H     | 6:Y:164:GLN:HB2  | 1.84                     | 0.41              |
| 8:L:-10:DT:H2"    | 8:L:-9:DC:C5     | 2.55                     | 0.41              |
| 1:a:175:LEU:HG    | 1:a:301:PHE:CZ   | 2.56                     | 0.41              |
| 1:c:298:LYS:HE2   | 1:d:232:PHE:O    | 2.20                     | 0.41              |
| 2:A:5:ILE:HD11    | 2:A:27:LEU:HD13  | 2.03                     | 0.41              |
| 3:U:102:LEU:HD13  | 3:U:115:ILE:HG22 | 2.02                     | 0.41              |
| 5:X:14:ASP:OD1    | 5:X:15:PHE:N     | 2.54                     | 0.41              |
| 5:X:1329:GLU:OE2  | 6:Y:331:ILE:HD11 | 2.21                     | 0.41              |
| 1:f:28:ARG:NH1    | 2:A:173:PHE:O    | 2.54                     | 0.41              |
| 1:a:296:ARG:HB2   | 1:a:297:PRO:HD3  | 2.03                     | 0.41              |
| 2:A:62:TRP:H      | 2:A:92:TYR:HD1   | 1.68                     | 0.41              |
| 2:A:170:ARG:NH2   | 2:A:231:GLY:O    | 2.54                     | 0.41              |
| 2:A:417:ILE:O     | 2:A:421:GLN:HG2  | 2.21                     | 0.41              |
| 3:V:30:PRO:C      | 3:V:31:LEU:HD12  | 2.46                     | 0.41              |
| 3:V:248:GLU:O     | 3:V:320:ASN:ND2  | 2.46                     | 0.41              |
| 5:X:214:ASN:OD1   | 5:X:359:ARG:NE   | 2.53                     | 0.41              |
| 5:X:233:ARG:HG3   | 5:X:234:ASP:OD1  | 2.20                     | 0.41              |
| 5:X:245:ARG:HD3   | 5:X:337:PHE:CD1  | 2.55                     | 0.41              |
| 5:X:445:ILE:HD12  | 5:X:445:ILE:HA   | 1.94                     | 0.41              |
| 5:X:575:LEU:HG    | 5:X:579:ALA:HB3  | 2.03                     | 0.41              |
| 5:X:646:SER:OG    | 5:X:647:ARG:N    | 2.54                     | 0.41              |
| 5:X:897:PRO:HA    | 5:X:900:LYS:HB2  | 2.03                     | 0.41              |
| 6:Y:225:GLU:HA    | 6:Y:228:VAL:HG12 | 2.01                     | 0.41              |
| 6:Y:399:LYS:O     | 6:Y:402:GLU:HG3  | 2.21                     | 0.41              |
| 6:Y:514:THR:HG21  | 6:Y:596:LEU:HG   | 2.03                     | 0.41              |
| 6:Y:649:LYS:HE3   | 6:Y:653:ILE:HD11 | 2.02                     | 0.41              |
| 6:Y:650:LYS:O     | 6:Y:651:HIS:C    | 2.62                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Y:801:VAL:O     | 6:Y:805:GLN:HG3   | 2.20                     | 0.41              |
| 1:f:28:ARG:HG2    | 2:A:172:ASN:HB3   | 2.01                     | 0.41              |
| 1:b:175:LEU:HG    | 1:b:301:PHE:CZ    | 2.56                     | 0.41              |
| 1:d:175:LEU:HG    | 1:d:301:PHE:CZ    | 2.56                     | 0.41              |
| 1:d:412:PHE:O     | 1:d:415:MET:HG2   | 2.20                     | 0.41              |
| 2:A:27:LEU:O      | 2:A:31:LEU:HG     | 2.21                     | 0.41              |
| 2:A:131:ARG:HG3   | 2:A:186:VAL:HG21  | 2.02                     | 0.41              |
| 3:V:302:GLU:O     | 3:V:306:VAL:HG22  | 2.21                     | 0.41              |
| 5:X:148:GLN:NE2   | 5:X:533:LEU:O     | 2.35                     | 0.41              |
| 6:Y:744:ARG:HH21  | 6:Y:767:LEU:HD21  | 1.84                     | 0.41              |
| 1:d:100:LYS:HD2   | 1:d:115:LYS:HE2   | 2.03                     | 0.40              |
| 1:e:296:ARG:HB2   | 1:e:297:PRO:HD3   | 2.03                     | 0.40              |
| 2:A:24:PHE:CD2    | 2:A:51:ARG:HG3    | 2.56                     | 0.40              |
| 5:X:559:CYS:CB    | 5:X:662:SER:HB3   | 2.51                     | 0.40              |
| 6:Y:1367:GLN:HB3  | 6:Y:1371:ARG:HH21 | 1.86                     | 0.40              |
| 1:f:138:PRO:HD2   | 1:a:217:THR:HG21  | 2.03                     | 0.40              |
| 1:b:100:LYS:HD2   | 1:b:115:LYS:HE2   | 2.03                     | 0.40              |
| 1:c:88:ARG:NH2    | 5:X:998:LEU:HD22  | 2.36                     | 0.40              |
| 1:e:175:LEU:HG    | 1:e:301:PHE:CZ    | 2.56                     | 0.40              |
| 3:U:33:ARG:HA     | 3:U:33:ARG:HD3    | 1.96                     | 0.40              |
| 3:U:214:GLU:O     | 3:U:218:ARG:HG2   | 2.21                     | 0.40              |
| 5:X:1194:GLU:O    | 5:X:1197:GLU:HG2  | 2.21                     | 0.40              |
| 5:X:1337:ILE:HG22 | 6:Y:22:ILE:HA     | 2.03                     | 0.40              |
| 6:Y:429:LEU:HD23  | 6:Y:429:LEU:HA    | 1.92                     | 0.40              |
| 1:f:6:LEU:O       | 1:f:9:THR:OG1     | 2.31                     | 0.40              |
| 1:a:173:ARG:HH21  | 1:b:212:ARG:HB3   | 1.86                     | 0.40              |
| 1:a:290:ASP:HB3   | 1:a:293:ALA:HB2   | 2.02                     | 0.40              |
| 1:a:390:MET:HB3   | 1:a:395:ALA:HB2   | 2.03                     | 0.40              |
| 1:d:6:LEU:O       | 1:d:9:THR:OG1     | 2.31                     | 0.40              |
| 2:A:295:SER:OG    | 2:A:345:GLN:O     | 2.23                     | 0.40              |
| 3:U:49:SER:OG     | 3:U:50:SER:N      | 2.53                     | 0.40              |
| 5:X:53:PHE:O      | 5:X:57:PHE:HB2    | 2.20                     | 0.40              |
| 5:X:367:TYR:HA    | 5:X:370:MET:HE3   | 2.03                     | 0.40              |
| 5:X:909:LYS:HA    | 5:X:909:LYS:HD3   | 1.94                     | 0.40              |
| 1:f:29:MET:HE2    | 1:f:29:MET:HB2    | 1.93                     | 0.40              |
| 1:f:296:ARG:HB2   | 1:f:297:PRO:HD3   | 2.03                     | 0.40              |
| 1:a:139:LEU:HD21  | 1:b:221:ARG:NH2   | 2.36                     | 0.40              |
| 1:b:92:ARG:NH2    | 1:b:132:LEU:HD22  | 2.37                     | 0.40              |
| 1:d:375:GLU:HA    | 1:d:375:GLU:OE2   | 2.22                     | 0.40              |
| 5:X:802:VAL:HG21  | 5:X:1230:MET:HB3  | 2.03                     | 0.40              |
| 5:X:806:PRO:HA    | 5:X:811:ASN:HD21  | 1.86                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:Y:269:TYR:HA   | 6:Y:272:VAL:HG12  | 2.03                     | 0.40              |
| 6:Y:857:LEU:HG   | 6:Y:858:VAL:HG23  | 2.02                     | 0.40              |
| 8:L:2:DG:H2"     | 8:L:3:DC:OP1      | 2.19                     | 0.40              |
| 1:f:175:LEU:HG   | 1:f:301:PHE:CZ    | 2.56                     | 0.40              |
| 1:a:70:SER:OG    | 1:a:73:LEU:HB2    | 2.22                     | 0.40              |
| 1:b:29:MET:HE2   | 1:b:29:MET:HB2    | 1.93                     | 0.40              |
| 1:b:296:ARG:HB2  | 1:b:297:PRO:HD3   | 2.03                     | 0.40              |
| 1:c:92:ARG:NH2   | 1:c:132:LEU:HD22  | 2.37                     | 0.40              |
| 1:c:173:ARG:NH2  | 1:d:212:ARG:HB3   | 2.36                     | 0.40              |
| 1:c:175:LEU:HG   | 1:c:301:PHE:CZ    | 2.56                     | 0.40              |
| 1:d:201:ASP:OD1  | 1:d:201:ASP:N     | 2.47                     | 0.40              |
| 1:e:100:LYS:HD2  | 1:e:115:LYS:HE2   | 2.04                     | 0.40              |
| 1:e:173:ARG:HD2  | 1:e:301:PHE:CE2   | 2.57                     | 0.40              |
| 1:e:375:GLU:HA   | 1:e:375:GLU:OE2   | 2.22                     | 0.40              |
| 2:A:203:GLU:O    | 2:A:207:GLU:HG2   | 2.21                     | 0.40              |
| 5:X:559:CYS:HA   | 5:X:560:PRO:HD3   | 1.91                     | 0.40              |
| 5:X:1149:TYR:HD2 | 5:X:1161:LEU:HD21 | 1.87                     | 0.40              |
| 6:Y:412:LEU:O    | 6:Y:416:ILE:HG12  | 2.21                     | 0.40              |
| 6:Y:673:VAL:HB   | 6:Y:677:GLU:HG3   | 2.03                     | 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     | 415/419 (99%) | 404 (97%) | 11 (3%) | 0        | 100         | 100 |
| 1   | b     | 415/419 (99%) | 404 (97%) | 11 (3%) | 0        | 100         | 100 |
| 1   | c     | 415/419 (99%) | 404 (97%) | 11 (3%) | 0        | 100         | 100 |
| 1   | d     | 415/419 (99%) | 404 (97%) | 11 (3%) | 0        | 100         | 100 |
| 1   | e     | 415/419 (99%) | 404 (97%) | 11 (3%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 1   | f     | 415/419 (99%)    | 404 (97%)  | 11 (3%)  | 0        | 100         | 100 |
| 2   | A     | 493/497 (99%)    | 454 (92%)  | 38 (8%)  | 1 (0%)   | 43          | 77  |
| 3   | U     | 233/329 (71%)    | 222 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| 3   | V     | 319/329 (97%)    | 295 (92%)  | 24 (8%)  | 0        | 100         | 100 |
| 4   | W     | 77/91 (85%)      | 75 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 5   | X     | 1338/1342 (100%) | 1274 (95%) | 64 (5%)  | 0        | 100         | 100 |
| 6   | Y     | 1356/1416 (96%)  | 1294 (95%) | 62 (5%)  | 0        | 100         | 100 |
| All | All   | 6306/6518 (97%)  | 6038 (96%) | 267 (4%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 200 | SER  |

### 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     | 357/359 (99%)    | 326 (91%)   | 31 (9%)  | 9           | 30  |
| 1   | b     | 357/359 (99%)    | 326 (91%)   | 31 (9%)  | 9           | 30  |
| 1   | c     | 357/359 (99%)    | 326 (91%)   | 31 (9%)  | 9           | 30  |
| 1   | d     | 357/359 (99%)    | 326 (91%)   | 31 (9%)  | 9           | 30  |
| 1   | e     | 357/359 (99%)    | 326 (91%)   | 31 (9%)  | 9           | 30  |
| 1   | f     | 357/359 (99%)    | 326 (91%)   | 31 (9%)  | 9           | 30  |
| 2   | A     | 409/409 (100%)   | 409 (100%)  | 0        | 100         | 100 |
| 3   | U     | 203/286 (71%)    | 203 (100%)  | 0        | 100         | 100 |
| 3   | V     | 280/286 (98%)    | 280 (100%)  | 0        | 100         | 100 |
| 4   | W     | 67/75 (89%)      | 67 (100%)   | 0        | 100         | 100 |
| 5   | X     | 1155/1157 (100%) | 1155 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 6   | Y     | 1134/1177 (96%) | 1134 (100%) | 0        | 100         | 100 |
| All | All   | 5390/5544 (97%) | 5204 (96%)  | 186 (4%) | 32          | 54  |

All (186) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | f     | 11  | VAL  |
| 1   | f     | 15  | ILE  |
| 1   | f     | 33  | ASP  |
| 1   | f     | 54  | VAL  |
| 1   | f     | 57  | ILE  |
| 1   | f     | 67  | SER  |
| 1   | f     | 71  | SER  |
| 1   | f     | 82  | SER  |
| 1   | f     | 106 | GLU  |
| 1   | f     | 114 | LEU  |
| 1   | f     | 117 | ASN  |
| 1   | f     | 137 | THR  |
| 1   | f     | 162 | LEU  |
| 1   | f     | 164 | LEU  |
| 1   | f     | 166 | SER  |
| 1   | f     | 181 | LYS  |
| 1   | f     | 194 | SER  |
| 1   | f     | 206 | VAL  |
| 1   | f     | 217 | THR  |
| 1   | f     | 228 | VAL  |
| 1   | f     | 245 | MET  |
| 1   | f     | 260 | VAL  |
| 1   | f     | 268 | THR  |
| 1   | f     | 276 | THR  |
| 1   | f     | 284 | VAL  |
| 1   | f     | 286 | THR  |
| 1   | f     | 326 | LYS  |
| 1   | f     | 343 | LEU  |
| 1   | f     | 373 | THR  |
| 1   | f     | 375 | GLU  |
| 1   | f     | 383 | LEU  |
| 1   | a     | 11  | VAL  |
| 1   | a     | 15  | ILE  |
| 1   | a     | 33  | ASP  |
| 1   | a     | 54  | VAL  |
| 1   | a     | 57  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 67  | SER  |
| 1   | a     | 71  | SER  |
| 1   | a     | 82  | SER  |
| 1   | a     | 106 | GLU  |
| 1   | a     | 114 | LEU  |
| 1   | a     | 117 | ASN  |
| 1   | a     | 137 | THR  |
| 1   | a     | 162 | LEU  |
| 1   | a     | 164 | LEU  |
| 1   | a     | 166 | SER  |
| 1   | a     | 181 | LYS  |
| 1   | a     | 194 | SER  |
| 1   | a     | 206 | VAL  |
| 1   | a     | 217 | THR  |
| 1   | a     | 228 | VAL  |
| 1   | a     | 245 | MET  |
| 1   | a     | 260 | VAL  |
| 1   | a     | 268 | THR  |
| 1   | a     | 276 | THR  |
| 1   | a     | 284 | VAL  |
| 1   | a     | 286 | THR  |
| 1   | a     | 326 | LYS  |
| 1   | a     | 343 | LEU  |
| 1   | a     | 373 | THR  |
| 1   | a     | 375 | GLU  |
| 1   | a     | 383 | LEU  |
| 1   | b     | 11  | VAL  |
| 1   | b     | 15  | ILE  |
| 1   | b     | 33  | ASP  |
| 1   | b     | 54  | VAL  |
| 1   | b     | 57  | ILE  |
| 1   | b     | 67  | SER  |
| 1   | b     | 71  | SER  |
| 1   | b     | 82  | SER  |
| 1   | b     | 106 | GLU  |
| 1   | b     | 114 | LEU  |
| 1   | b     | 117 | ASN  |
| 1   | b     | 137 | THR  |
| 1   | b     | 162 | LEU  |
| 1   | b     | 164 | LEU  |
| 1   | b     | 166 | SER  |
| 1   | b     | 181 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 194 | SER  |
| 1   | b     | 206 | VAL  |
| 1   | b     | 217 | THR  |
| 1   | b     | 228 | VAL  |
| 1   | b     | 245 | MET  |
| 1   | b     | 260 | VAL  |
| 1   | b     | 268 | THR  |
| 1   | b     | 276 | THR  |
| 1   | b     | 284 | VAL  |
| 1   | b     | 286 | THR  |
| 1   | b     | 326 | LYS  |
| 1   | b     | 343 | LEU  |
| 1   | b     | 373 | THR  |
| 1   | b     | 375 | GLU  |
| 1   | b     | 383 | LEU  |
| 1   | c     | 11  | VAL  |
| 1   | c     | 15  | ILE  |
| 1   | c     | 33  | ASP  |
| 1   | c     | 54  | VAL  |
| 1   | c     | 57  | ILE  |
| 1   | c     | 67  | SER  |
| 1   | c     | 71  | SER  |
| 1   | c     | 82  | SER  |
| 1   | c     | 106 | GLU  |
| 1   | c     | 114 | LEU  |
| 1   | c     | 117 | ASN  |
| 1   | c     | 137 | THR  |
| 1   | c     | 162 | LEU  |
| 1   | c     | 164 | LEU  |
| 1   | c     | 166 | SER  |
| 1   | c     | 181 | LYS  |
| 1   | c     | 194 | SER  |
| 1   | c     | 206 | VAL  |
| 1   | c     | 217 | THR  |
| 1   | c     | 228 | VAL  |
| 1   | c     | 245 | MET  |
| 1   | c     | 260 | VAL  |
| 1   | c     | 268 | THR  |
| 1   | c     | 276 | THR  |
| 1   | c     | 284 | VAL  |
| 1   | c     | 286 | THR  |
| 1   | c     | 326 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | c     | 343 | LEU  |
| 1   | c     | 373 | THR  |
| 1   | c     | 375 | GLU  |
| 1   | c     | 383 | LEU  |
| 1   | d     | 11  | VAL  |
| 1   | d     | 15  | ILE  |
| 1   | d     | 33  | ASP  |
| 1   | d     | 54  | VAL  |
| 1   | d     | 57  | ILE  |
| 1   | d     | 67  | SER  |
| 1   | d     | 71  | SER  |
| 1   | d     | 82  | SER  |
| 1   | d     | 106 | GLU  |
| 1   | d     | 114 | LEU  |
| 1   | d     | 117 | ASN  |
| 1   | d     | 137 | THR  |
| 1   | d     | 162 | LEU  |
| 1   | d     | 164 | LEU  |
| 1   | d     | 166 | SER  |
| 1   | d     | 181 | LYS  |
| 1   | d     | 194 | SER  |
| 1   | d     | 206 | VAL  |
| 1   | d     | 217 | THR  |
| 1   | d     | 228 | VAL  |
| 1   | d     | 245 | MET  |
| 1   | d     | 260 | VAL  |
| 1   | d     | 268 | THR  |
| 1   | d     | 276 | THR  |
| 1   | d     | 284 | VAL  |
| 1   | d     | 286 | THR  |
| 1   | d     | 326 | LYS  |
| 1   | d     | 343 | LEU  |
| 1   | d     | 373 | THR  |
| 1   | d     | 375 | GLU  |
| 1   | d     | 383 | LEU  |
| 1   | e     | 11  | VAL  |
| 1   | e     | 15  | ILE  |
| 1   | e     | 33  | ASP  |
| 1   | e     | 54  | VAL  |
| 1   | e     | 57  | ILE  |
| 1   | e     | 67  | SER  |
| 1   | e     | 71  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | e     | 82  | SER  |
| 1   | e     | 106 | GLU  |
| 1   | e     | 114 | LEU  |
| 1   | e     | 117 | ASN  |
| 1   | e     | 137 | THR  |
| 1   | e     | 162 | LEU  |
| 1   | e     | 164 | LEU  |
| 1   | e     | 166 | SER  |
| 1   | e     | 181 | LYS  |
| 1   | e     | 194 | SER  |
| 1   | e     | 206 | VAL  |
| 1   | e     | 217 | THR  |
| 1   | e     | 228 | VAL  |
| 1   | e     | 245 | MET  |
| 1   | e     | 260 | VAL  |
| 1   | e     | 268 | THR  |
| 1   | e     | 276 | THR  |
| 1   | e     | 284 | VAL  |
| 1   | e     | 286 | THR  |
| 1   | e     | 326 | LYS  |
| 1   | e     | 343 | LEU  |
| 1   | e     | 373 | THR  |
| 1   | e     | 375 | GLU  |
| 1   | e     | 383 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | f     | 85  | GLN  |
| 1   | f     | 90  | ASN  |
| 1   | f     | 142 | ASN  |
| 1   | a     | 85  | GLN  |
| 1   | a     | 90  | ASN  |
| 1   | a     | 142 | ASN  |
| 1   | b     | 25  | ASN  |
| 1   | b     | 85  | GLN  |
| 1   | b     | 90  | ASN  |
| 1   | b     | 140 | HIS  |
| 1   | b     | 142 | ASN  |
| 1   | c     | 85  | GLN  |
| 1   | c     | 90  | ASN  |
| 1   | c     | 142 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | d     | 85   | GLN  |
| 1   | d     | 90   | ASN  |
| 1   | d     | 142  | ASN  |
| 1   | e     | 85   | GLN  |
| 1   | e     | 90   | ASN  |
| 1   | e     | 142  | ASN  |
| 2   | A     | 14   | ASN  |
| 2   | A     | 116  | GLN  |
| 2   | A     | 129  | GLN  |
| 2   | A     | 157  | ASN  |
| 2   | A     | 282  | GLN  |
| 2   | A     | 324  | ASN  |
| 2   | A     | 330  | GLN  |
| 2   | A     | 487  | ASN  |
| 3   | V     | 132  | HIS  |
| 3   | V     | 194  | GLN  |
| 3   | V     | 239  | GLN  |
| 3   | V     | 283  | GLN  |
| 5   | X     | 238  | GLN  |
| 5   | X     | 343  | HIS  |
| 5   | X     | 519  | ASN  |
| 5   | X     | 580  | GLN  |
| 5   | X     | 799  | ASN  |
| 5   | X     | 808  | ASN  |
| 5   | X     | 932  | GLN  |
| 5   | X     | 1009 | ASN  |
| 5   | X     | 1010 | GLN  |
| 5   | X     | 1013 | GLN  |
| 5   | X     | 1017 | GLN  |
| 5   | X     | 1136 | GLN  |
| 5   | X     | 1209 | GLN  |
| 6   | Y     | 196  | GLN  |
| 6   | Y     | 209  | ASN  |
| 6   | Y     | 266  | ASN  |
| 6   | Y     | 341  | ASN  |
| 6   | Y     | 365  | GLN  |
| 6   | Y     | 435  | GLN  |
| 6   | Y     | 488  | ASN  |
| 6   | Y     | 545  | HIS  |
| 6   | Y     | 739  | GLN  |
| 6   | Y     | 805  | GLN  |
| 6   | Y     | 865  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | Y     | 897  | HIS  |
| 6   | Y     | 921  | GLN  |
| 6   | Y     | 954  | ASN  |
| 6   | Y     | 968  | ASN  |
| 6   | Y     | 1023 | HIS  |
| 6   | Y     | 1197 | ASN  |
| 6   | Y     | 1244 | GLN  |
| 6   | Y     | 1268 | ASN  |
| 6   | Y     | 1326 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 9   | R     | 26/99 (26%) | 8 (30%)           | 0               |

All (8) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | R     | 23  | U    |
| 9   | R     | 24  | U    |
| 9   | R     | 25  | C    |
| 9   | R     | 84  | A    |
| 9   | R     | 86  | A    |
| 9   | R     | 88  | C    |
| 9   | R     | 90  | G    |
| 9   | R     | 92  | C    |

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 12  | BEF  | c     | 504  | -    | 0,3,3        | -    | -        | -           |      |          |
| 10  | ADP  | b     | 1000 | 1,11 | 27,29,29     | 1.36 | 4 (14%)  | 42,45,45    | 1.96 | 11 (26%) |
| 10  | ADP  | d     | 1000 | 1,11 | 27,29,29     | 1.36 | 4 (14%)  | 42,45,45    | 1.95 | 11 (26%) |
| 10  | ADP  | e     | 1000 | 11   | 27,29,29     | 1.36 | 4 (14%)  | 42,45,45    | 1.97 | 10 (23%) |
| 12  | BEF  | e     | 1002 | -    | 0,3,3        | -    | -        | -           |      |          |
| 12  | BEF  | a     | 1002 | -    | 0,3,3        | -    | -        | -           |      |          |
| 10  | ADP  | c     | 501  | 1,11 | 27,29,29     | 1.35 | 4 (14%)  | 42,45,45    | 1.94 | 11 (26%) |
| 12  | BEF  | c     | 503  | -    | 0,3,3        | -    | -        | -           |      |          |
| 10  | ADP  | a     | 1000 | 11   | 27,29,29     | 1.35 | 4 (14%)  | 42,45,45    | 1.98 | 10 (23%) |
| 12  | BEF  | b     | 1002 | -    | 0,3,3        | -    | -        | -           |      |          |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 10  | ADP  | b     | 1000 | 1,11 | -       | 5/16/32/32 | 0/3/3/3 |
| 10  | ADP  | d     | 1000 | 1,11 | -       | 3/16/32/32 | 0/3/3/3 |
| 10  | ADP  | e     | 1000 | 11   | -       | 2/16/32/32 | 0/3/3/3 |
| 10  | ADP  | c     | 501  | 1,11 | -       | 6/16/32/32 | 0/3/3/3 |
| 10  | ADP  | a     | 1000 | 11   | -       | 0/16/32/32 | 0/3/3/3 |

All (20) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 10  | e     | 1000 | ADP  | C5-C4 | 4.58 | 1.47        | 1.39     |
| 10  | a     | 1000 | ADP  | C5-C4 | 4.55 | 1.47        | 1.39     |
| 10  | b     | 1000 | ADP  | C5-C4 | 4.53 | 1.47        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 10  | d     | 1000 | ADP  | C5-C4 | 4.49  | 1.47        | 1.39     |
| 10  | c     | 501  | ADP  | C5-C4 | 4.49  | 1.47        | 1.39     |
| 10  | d     | 1000 | ADP  | C5-C6 | 2.69  | 1.48        | 1.41     |
| 10  | c     | 501  | ADP  | C5-C6 | 2.69  | 1.48        | 1.41     |
| 10  | e     | 1000 | ADP  | C5-C6 | 2.67  | 1.48        | 1.41     |
| 10  | b     | 1000 | ADP  | C5-C6 | 2.66  | 1.48        | 1.41     |
| 10  | a     | 1000 | ADP  | C5-C6 | 2.65  | 1.48        | 1.41     |
| 10  | d     | 1000 | ADP  | C8-N7 | 2.41  | 1.36        | 1.31     |
| 10  | e     | 1000 | ADP  | C8-N7 | 2.41  | 1.36        | 1.31     |
| 10  | b     | 1000 | ADP  | C8-N7 | 2.39  | 1.36        | 1.31     |
| 10  | c     | 501  | ADP  | C8-N7 | 2.39  | 1.36        | 1.31     |
| 10  | a     | 1000 | ADP  | C8-N7 | 2.32  | 1.36        | 1.31     |
| 10  | c     | 501  | ADP  | C5-N7 | -2.20 | 1.34        | 1.39     |
| 10  | b     | 1000 | ADP  | C5-N7 | -2.19 | 1.34        | 1.39     |
| 10  | e     | 1000 | ADP  | C5-N7 | -2.18 | 1.34        | 1.39     |
| 10  | a     | 1000 | ADP  | C5-N7 | -2.16 | 1.34        | 1.39     |
| 10  | d     | 1000 | ADP  | C5-N7 | -2.13 | 1.35        | 1.39     |

All (53) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 10  | a     | 1000 | ADP  | C5-C4-N3  | -6.33 | 118.49      | 126.75   |
| 10  | b     | 1000 | ADP  | C5-C4-N3  | -6.16 | 118.71      | 126.75   |
| 10  | e     | 1000 | ADP  | C5-C4-N3  | -6.16 | 118.71      | 126.75   |
| 10  | c     | 501  | ADP  | C5-C4-N3  | -6.15 | 118.73      | 126.75   |
| 10  | d     | 1000 | ADP  | C5-C4-N3  | -6.08 | 118.81      | 126.75   |
| 10  | a     | 1000 | ADP  | N3-C4-N9  | 4.95  | 135.23      | 127.08   |
| 10  | e     | 1000 | ADP  | N3-C4-N9  | 4.86  | 135.09      | 127.08   |
| 10  | c     | 501  | ADP  | N3-C4-N9  | 4.86  | 135.09      | 127.08   |
| 10  | b     | 1000 | ADP  | N3-C4-N9  | 4.86  | 135.08      | 127.08   |
| 10  | d     | 1000 | ADP  | N3-C4-N9  | 4.80  | 134.99      | 127.08   |
| 10  | a     | 1000 | ADP  | C2-N3-C4  | 3.88  | 120.92      | 111.75   |
| 10  | b     | 1000 | ADP  | C2-N3-C4  | 3.85  | 120.84      | 111.75   |
| 10  | e     | 1000 | ADP  | C2-N3-C4  | 3.83  | 120.80      | 111.75   |
| 10  | c     | 501  | ADP  | C2-N3-C4  | 3.83  | 120.80      | 111.75   |
| 10  | d     | 1000 | ADP  | C2-N3-C4  | 3.82  | 120.77      | 111.75   |
| 10  | a     | 1000 | ADP  | PA-O3A-PB | -3.70 | 120.13      | 132.83   |
| 10  | e     | 1000 | ADP  | PA-O3A-PB | -3.39 | 121.21      | 132.83   |
| 10  | a     | 1000 | ADP  | C4-C5-N7  | -3.22 | 106.70      | 110.62   |
| 10  | c     | 501  | ADP  | C4-C5-N7  | -3.22 | 106.70      | 110.62   |
| 10  | b     | 1000 | ADP  | C4-C5-N7  | -3.21 | 106.71      | 110.62   |
| 10  | d     | 1000 | ADP  | C4-C5-N7  | -3.21 | 106.71      | 110.62   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 10  | e     | 1000 | ADP  | C4-C5-N7    | -3.20 | 106.72      | 110.62   |
| 10  | e     | 1000 | ADP  | N3-C2-N1    | -3.12 | 123.72      | 128.60   |
| 10  | b     | 1000 | ADP  | N3-C2-N1    | -3.12 | 123.72      | 128.60   |
| 10  | d     | 1000 | ADP  | N3-C2-N1    | -3.11 | 123.73      | 128.60   |
| 10  | a     | 1000 | ADP  | N3-C2-N1    | -3.11 | 123.74      | 128.60   |
| 10  | c     | 501  | ADP  | N3-C2-N1    | -3.10 | 123.75      | 128.60   |
| 10  | d     | 1000 | ADP  | PA-O3A-PB   | -3.02 | 122.46      | 132.83   |
| 10  | c     | 501  | ADP  | C5-N7-C8    | 2.75  | 107.41      | 103.51   |
| 10  | b     | 1000 | ADP  | C5-N7-C8    | 2.72  | 107.38      | 103.51   |
| 10  | d     | 1000 | ADP  | C5-N7-C8    | 2.70  | 107.35      | 103.51   |
| 10  | e     | 1000 | ADP  | C5-N7-C8    | 2.70  | 107.34      | 103.51   |
| 10  | d     | 1000 | ADP  | C4-N9-C8    | 2.66  | 108.61      | 105.73   |
| 10  | c     | 501  | ADP  | C4-N9-C8    | 2.65  | 108.60      | 105.73   |
| 10  | a     | 1000 | ADP  | C5-N7-C8    | 2.64  | 107.26      | 103.51   |
| 10  | b     | 1000 | ADP  | C4-N9-C8    | 2.62  | 108.56      | 105.73   |
| 10  | b     | 1000 | ADP  | C3'-C2'-C1' | 2.58  | 106.34      | 101.43   |
| 10  | b     | 1000 | ADP  | PA-O3A-PB   | -2.57 | 124.00      | 132.83   |
| 10  | e     | 1000 | ADP  | C4-N9-C8    | 2.57  | 108.51      | 105.73   |
| 10  | c     | 501  | ADP  | C3'-C2'-C1' | 2.57  | 106.30      | 101.43   |
| 10  | a     | 1000 | ADP  | C3'-C2'-C1' | 2.55  | 106.26      | 101.43   |
| 10  | e     | 1000 | ADP  | C3'-C2'-C1' | 2.54  | 106.25      | 101.43   |
| 10  | d     | 1000 | ADP  | C3'-C2'-C1' | 2.50  | 106.17      | 101.43   |
| 10  | a     | 1000 | ADP  | C4-N9-C8    | 2.40  | 108.33      | 105.73   |
| 10  | c     | 501  | ADP  | PA-O3A-PB   | -2.29 | 124.98      | 132.83   |
| 10  | d     | 1000 | ADP  | C6-C5-N7    | 2.16  | 136.04      | 132.02   |
| 10  | b     | 1000 | ADP  | C6-C5-N7    | 2.16  | 136.04      | 132.02   |
| 10  | c     | 501  | ADP  | C6-C5-N7    | 2.12  | 135.97      | 132.02   |
| 10  | e     | 1000 | ADP  | C6-C5-N7    | 2.12  | 135.97      | 132.02   |
| 10  | a     | 1000 | ADP  | C6-C5-N7    | 2.07  | 135.87      | 132.02   |
| 10  | c     | 501  | ADP  | N9-C8-N7    | -2.06 | 111.10      | 113.91   |
| 10  | d     | 1000 | ADP  | N9-C8-N7    | -2.03 | 111.14      | 113.91   |
| 10  | b     | 1000 | ADP  | N9-C8-N7    | -2.02 | 111.14      | 113.91   |

There are no chirality outliers.

All (16) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 10  | b     | 1000 | ADP  | PA-O3A-PB-O2B  |
| 10  | b     | 1000 | ADP  | PA-O3A-PB-O3B  |
| 10  | b     | 1000 | ADP  | C5'-O5'-PA-O3A |
| 10  | c     | 501  | ADP  | C5'-O5'-PA-O1A |
| 10  | d     | 1000 | ADP  | PA-O3A-PB-O3B  |

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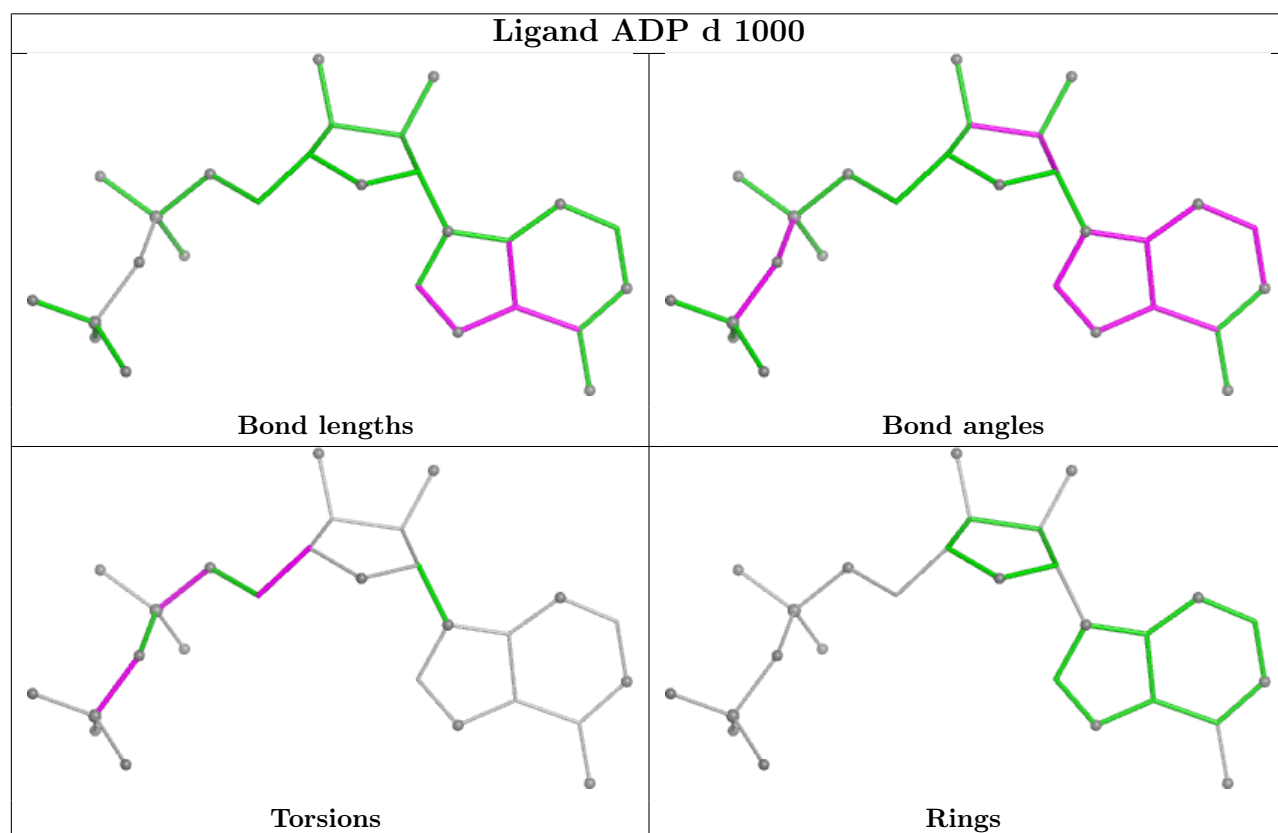
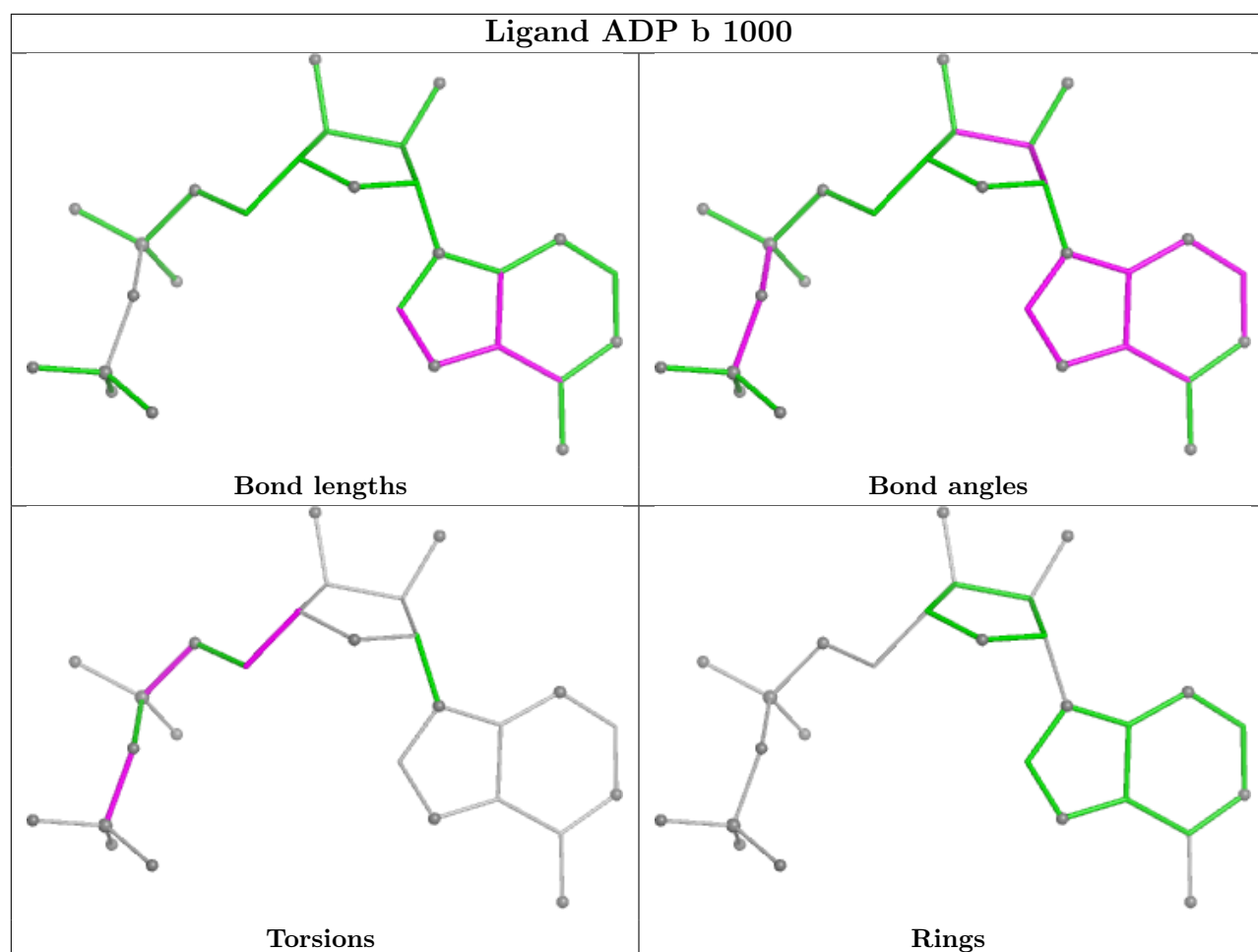
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 10  | c     | 501  | ADP  | C5'-O5'-PA-O3A  |
| 10  | b     | 1000 | ADP  | C5'-O5'-PA-O1A  |
| 10  | c     | 501  | ADP  | PA-O3A-PB-O1B   |
| 10  | c     | 501  | ADP  | O4'-C4'-C5'-O5' |
| 10  | c     | 501  | ADP  | PA-O3A-PB-O2B   |
| 10  | c     | 501  | ADP  | PA-O3A-PB-O3B   |
| 10  | d     | 1000 | ADP  | C5'-O5'-PA-O1A  |
| 10  | e     | 1000 | ADP  | C5'-O5'-PA-O1A  |
| 10  | b     | 1000 | ADP  | O4'-C4'-C5'-O5' |
| 10  | d     | 1000 | ADP  | O4'-C4'-C5'-O5' |
| 10  | e     | 1000 | ADP  | O4'-C4'-C5'-O5' |

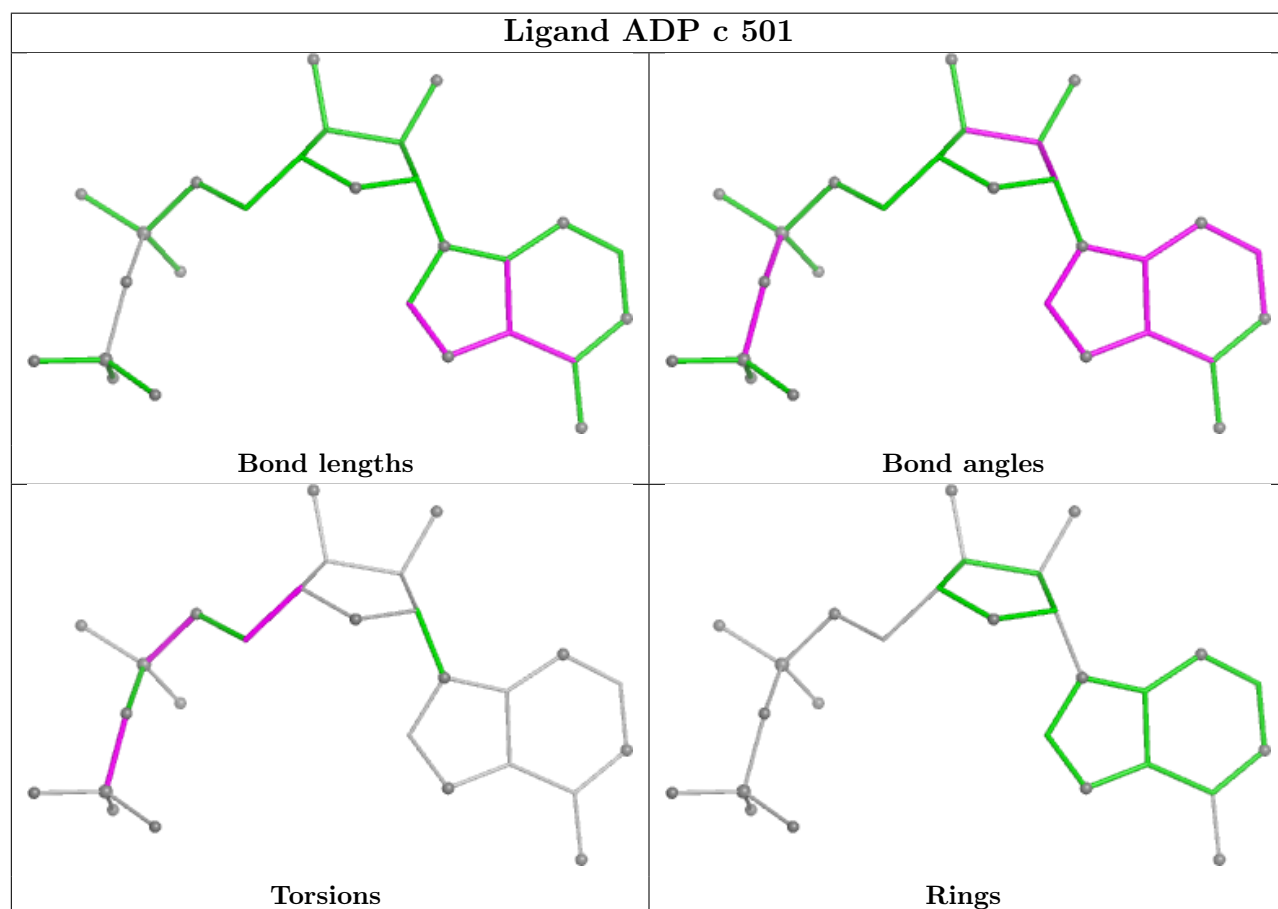
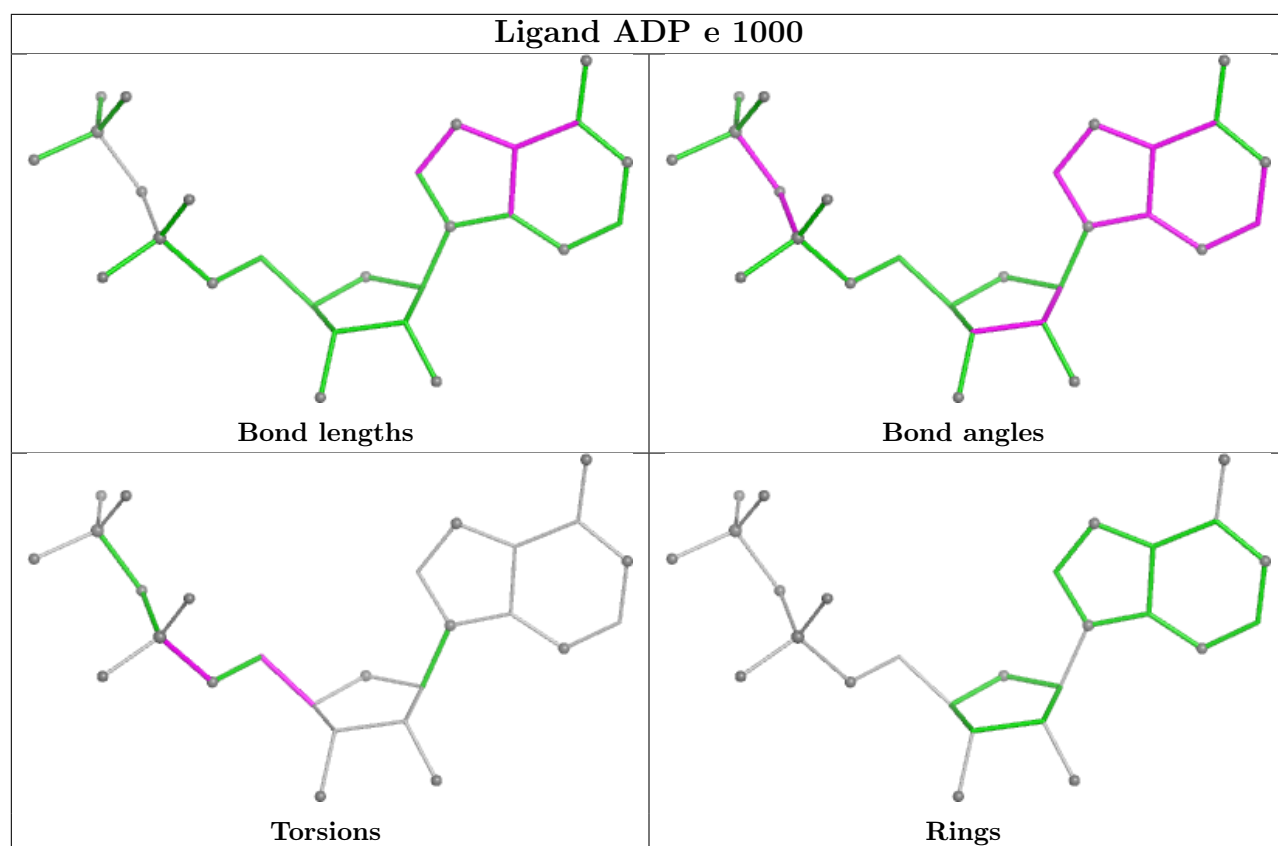
There are no ring outliers.

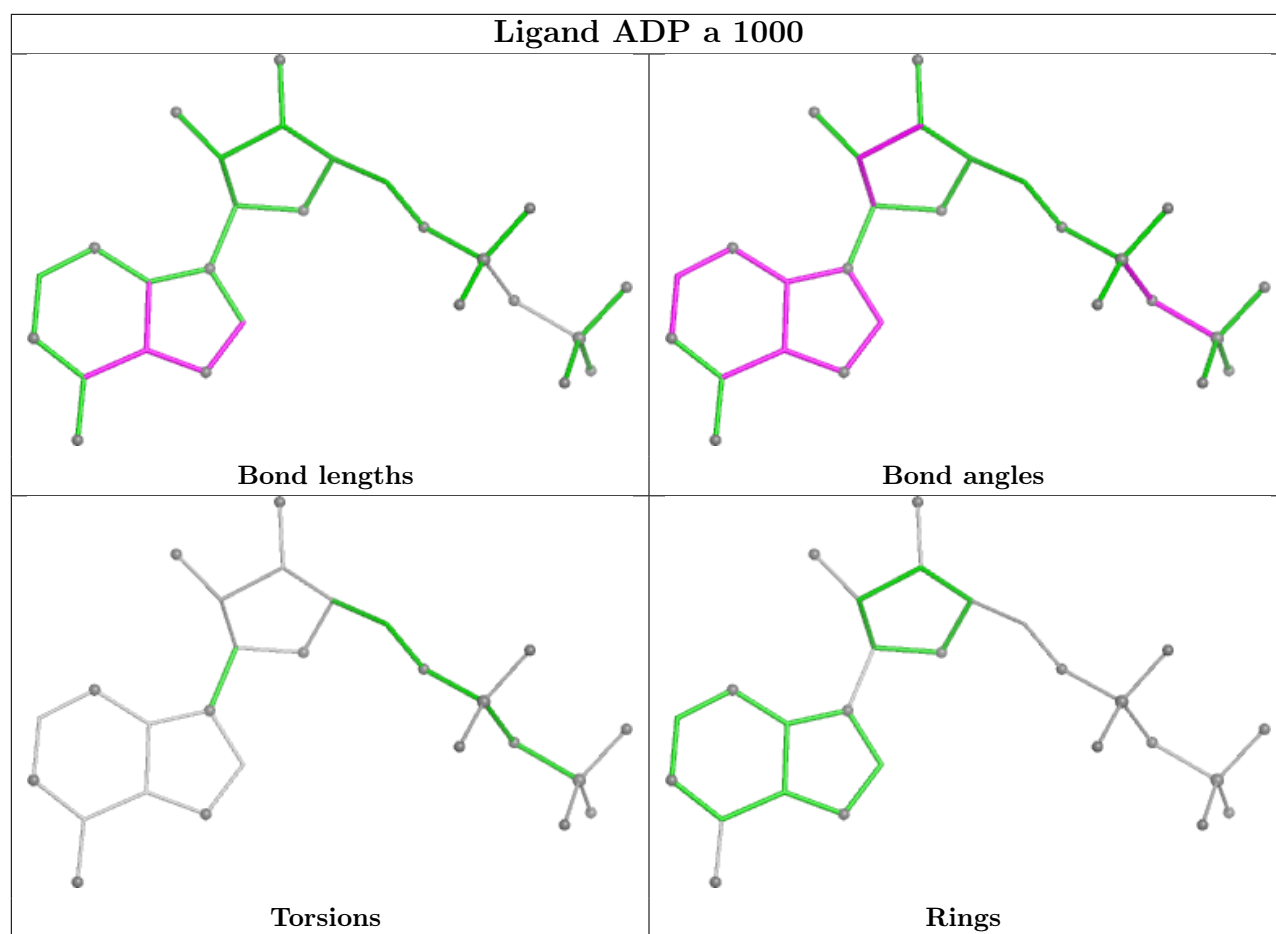
10 monomers are involved in 14 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 12  | c     | 504  | BEF  | 2       | 0            |
| 10  | b     | 1000 | ADP  | 2       | 0            |
| 10  | d     | 1000 | ADP  | 1       | 0            |
| 10  | e     | 1000 | ADP  | 3       | 0            |
| 12  | e     | 1002 | BEF  | 2       | 0            |
| 12  | a     | 1002 | BEF  | 1       | 0            |
| 10  | c     | 501  | ADP  | 1       | 0            |
| 12  | c     | 503  | BEF  | 2       | 0            |
| 10  | a     | 1000 | ADP  | 2       | 0            |
| 12  | b     | 1002 | BEF  | 3       | 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](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 8   | L     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | L     | -2:DC     | O3'    | -1:DA     | P      | 3.70         |

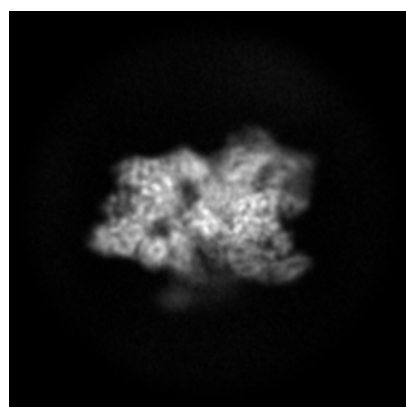
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11724. These allow visual inspection of the internal detail of the map and identification of artifacts.

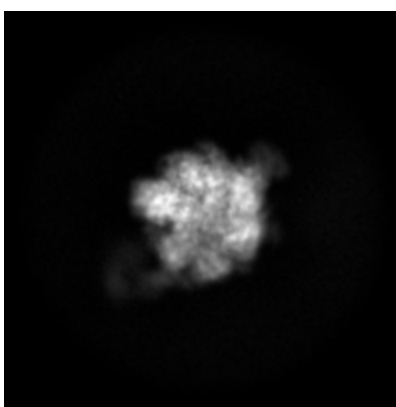
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

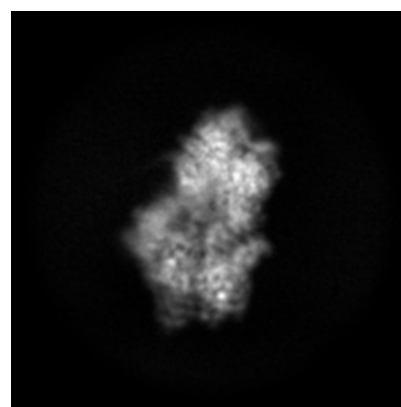
#### 6.1.1 Primary map



X



Y

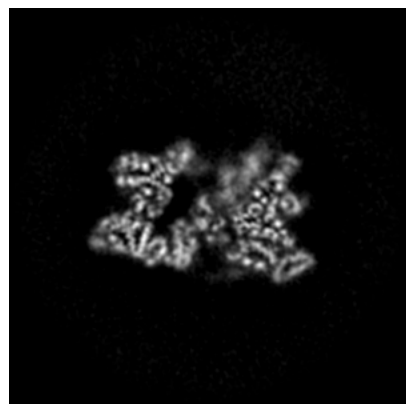


Z

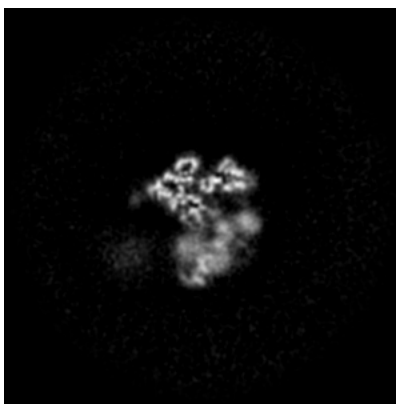
The images above show the map projected in three orthogonal directions.

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

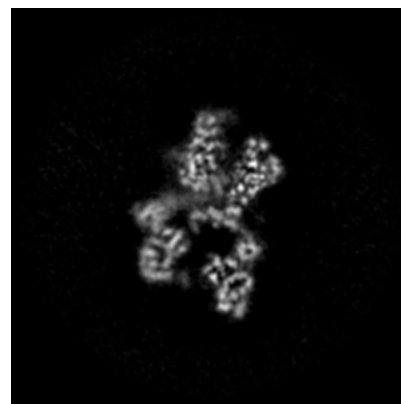
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

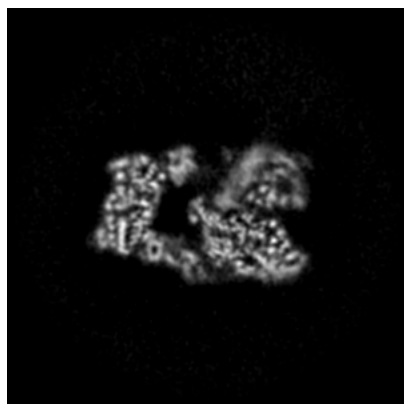


Z Index: 150

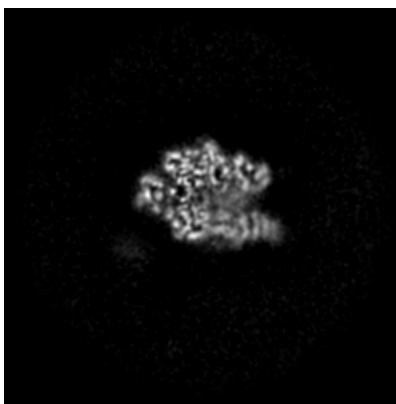
The images above show central slices of the map in three orthogonal directions.

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

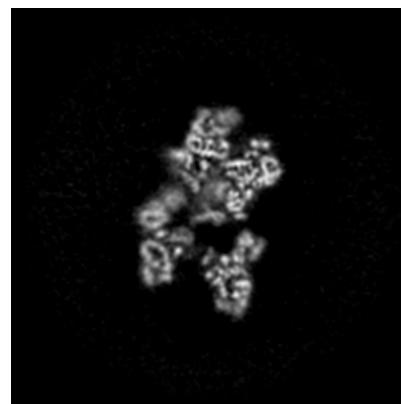
### 6.3.1 Primary map



X Index: 157



Y Index: 172

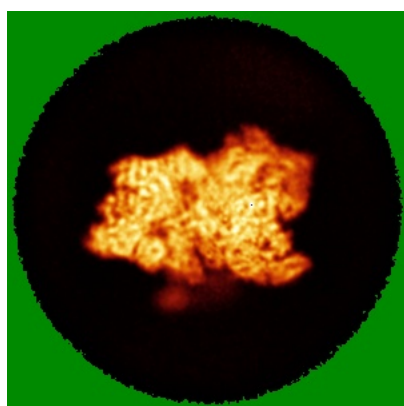


Z Index: 155

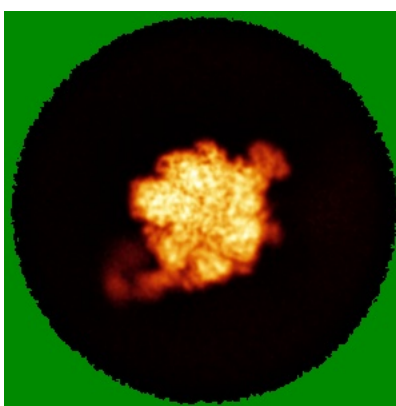
The images above show the largest variance slices of the map in three orthogonal directions.

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

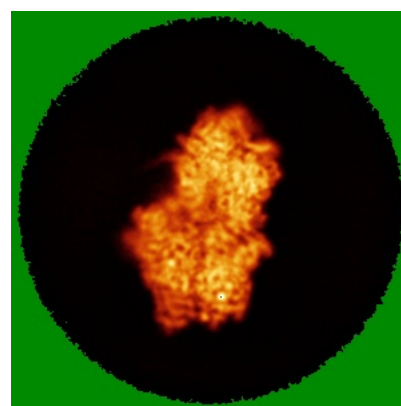
### 6.4.1 Primary map



X



Y

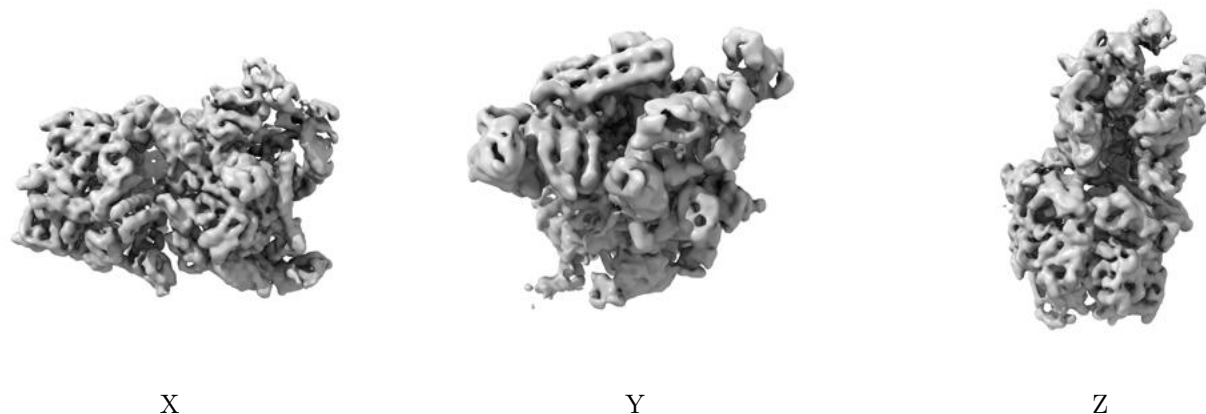


Z

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 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

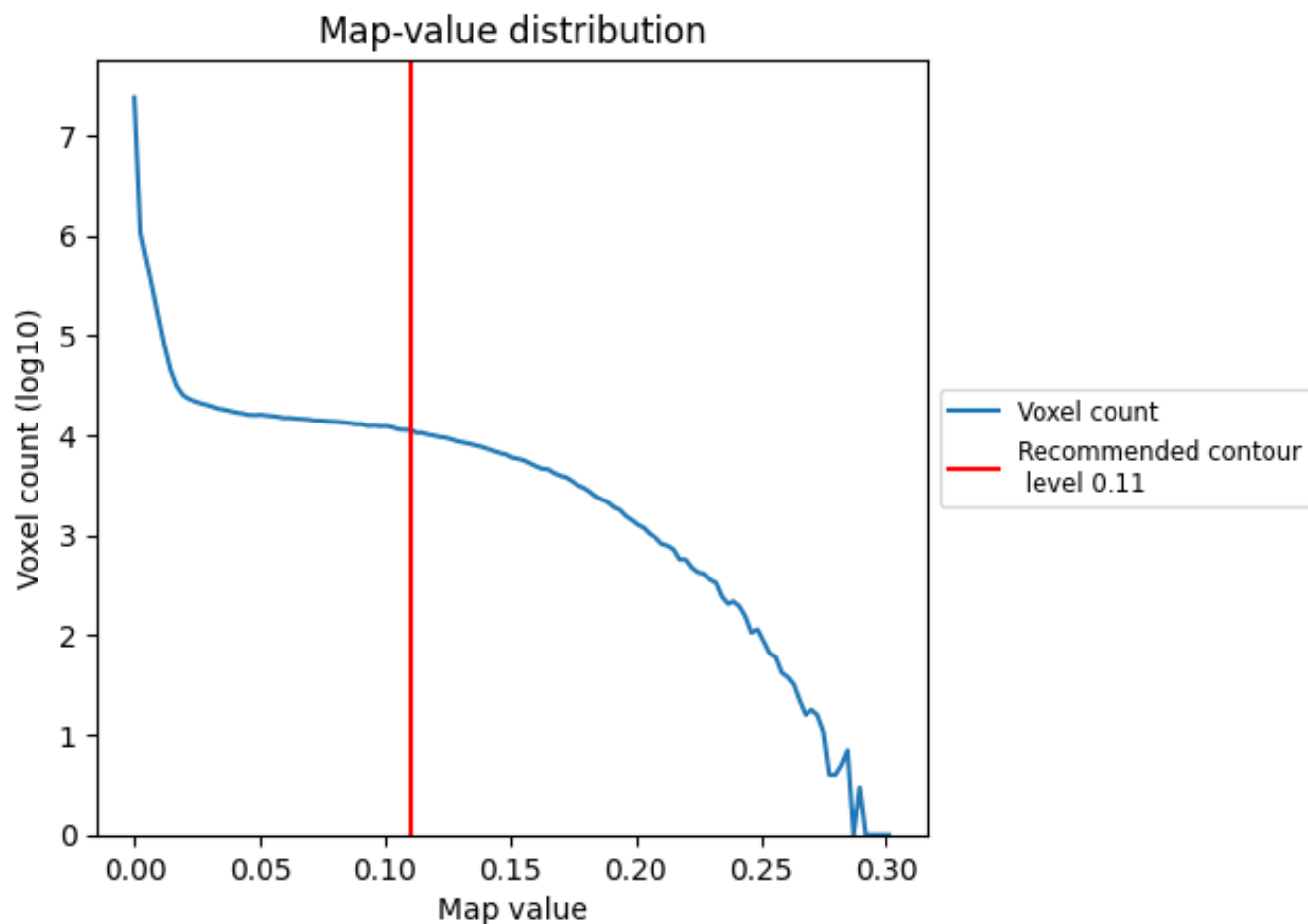
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

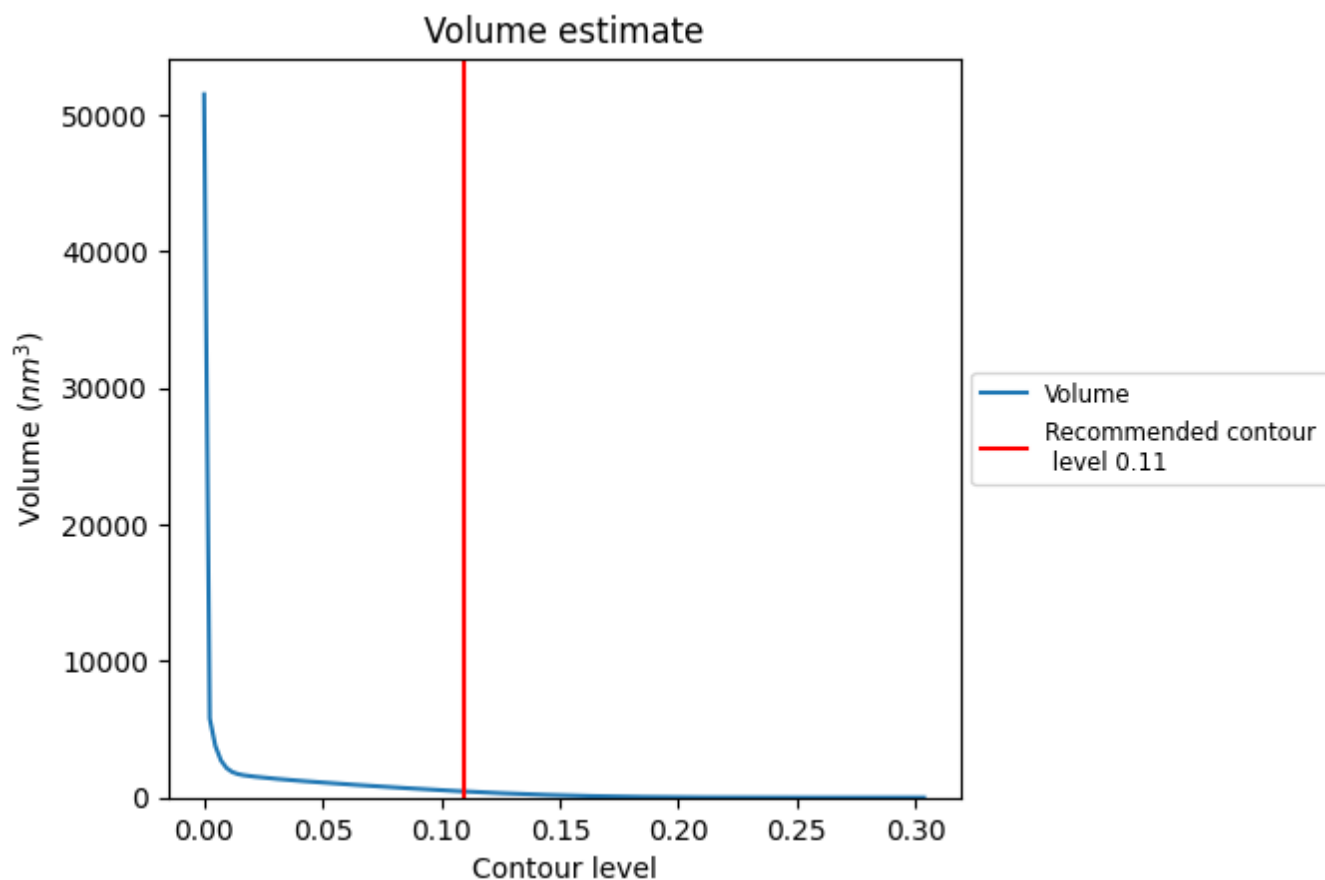
This section contains the results of statistical analysis of the map.

### 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.

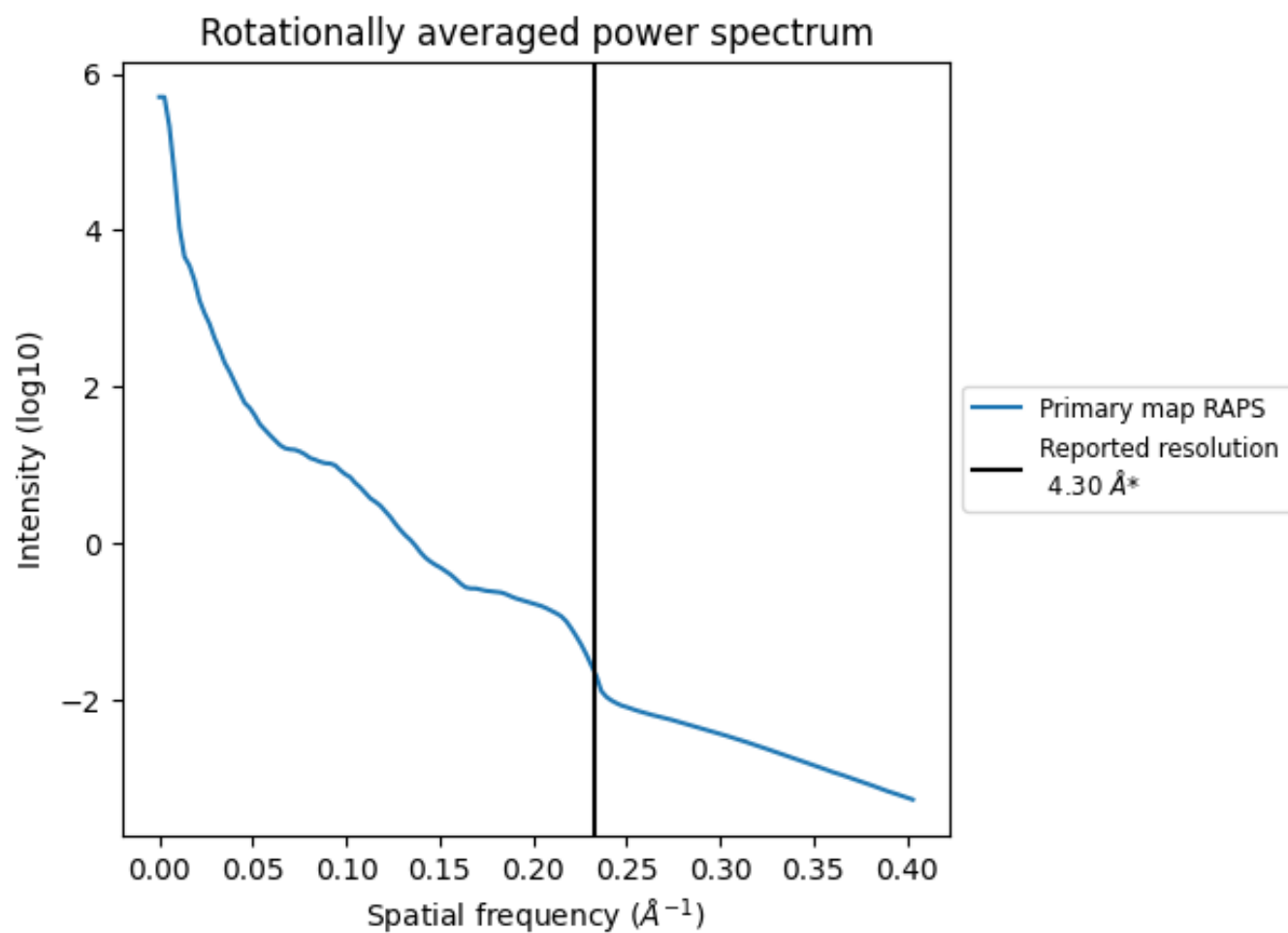
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 446  $\text{nm}^3$ ; this corresponds to an approximate mass of 403 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 ⓘ

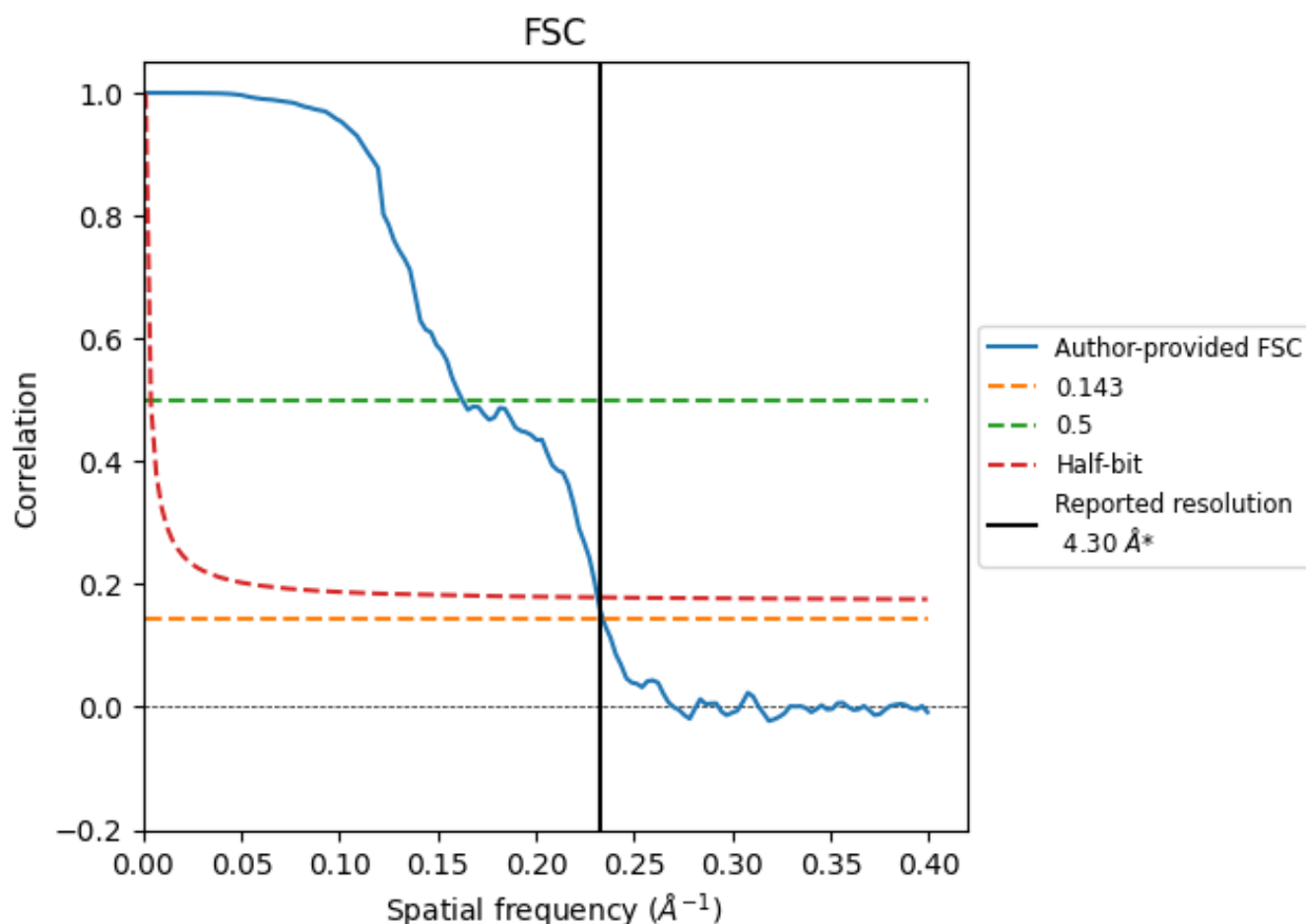


\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

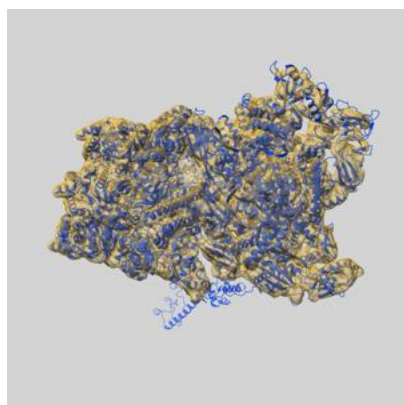
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.30                               | -    | -        |
| Author-provided FSC curve | 4.27                               | 6.16 | 4.32     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

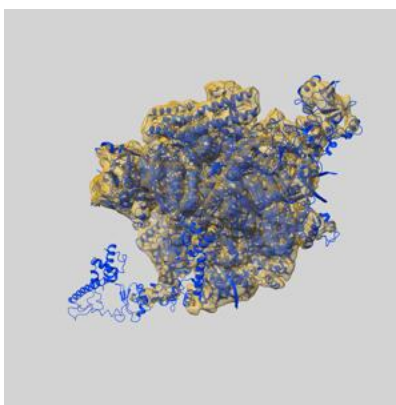
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11724 and PDB model 7ADD. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

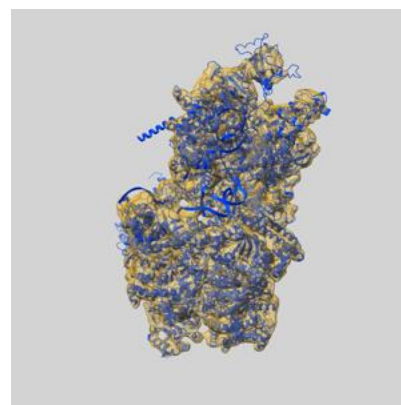
### 9.1 Map-model overlay [i](#)



X



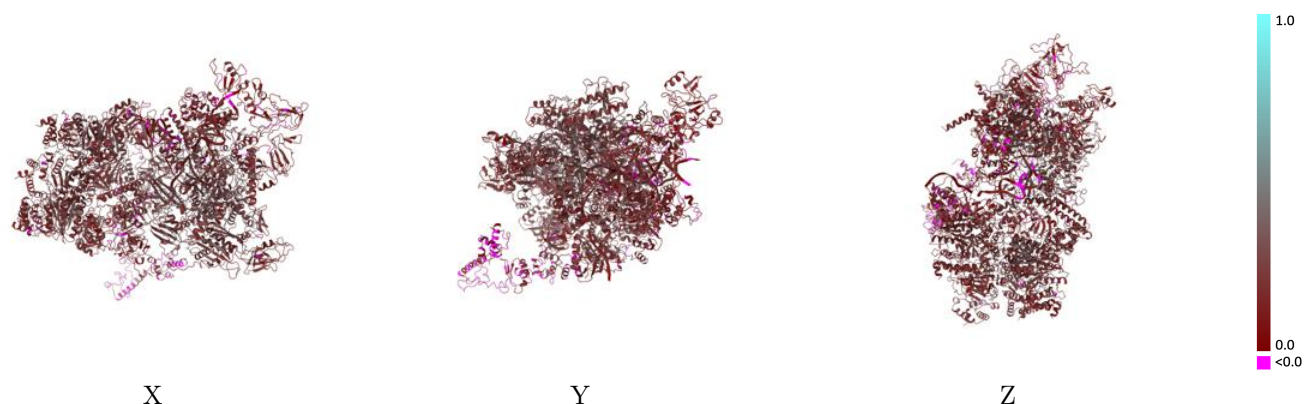
Y



Z

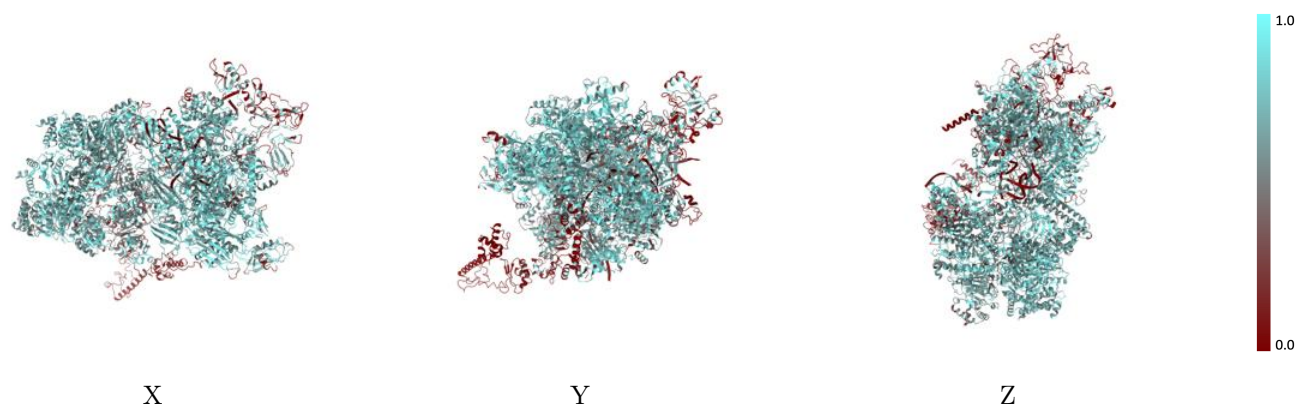
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



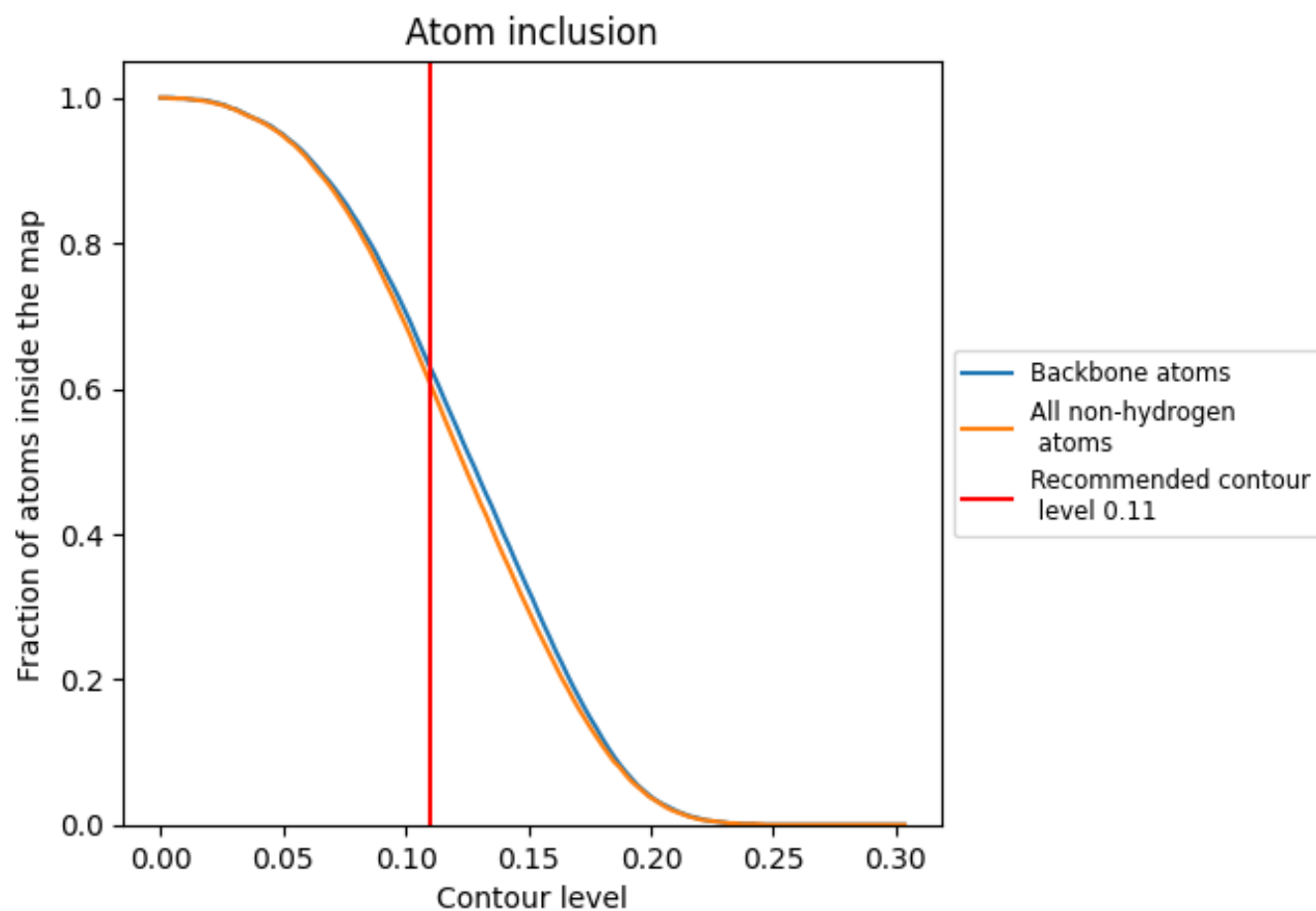
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.11).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 63% of all backbone atoms, 61% 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 (0.11) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.6070 | <div></div> 0.2170 |
| A     | <div></div> 0.2680 | <div></div> 0.1220 |
| K     | <div></div> 0.3850 | <div></div> 0.1190 |
| L     | <div></div> 0.4320 | <div></div> 0.1220 |
| R     | <div></div> 0.4410 | <div></div> 0.1530 |
| U     | <div></div> 0.6880 | <div></div> 0.2770 |
| V     | <div></div> 0.6170 | <div></div> 0.2330 |
| W     | <div></div> 0.0610 | <div></div> 0.2200 |
| X     | <div></div> 0.6880 | <div></div> 0.2610 |
| Y     | <div></div> 0.6070 | <div></div> 0.2120 |
| a     | <div></div> 0.6730 | <div></div> 0.2100 |
| b     | <div></div> 0.7300 | <div></div> 0.2320 |
| c     | <div></div> 0.7200 | <div></div> 0.2400 |
| d     | <div></div> 0.6970 | <div></div> 0.2310 |
| e     | <div></div> 0.6110 | <div></div> 0.1990 |
| f     | <div></div> 0.6310 | <div></div> 0.1830 |

1.0

0.0

<0.0