



## Full wwPDB EM Validation Report ⓘ

Aug 26, 2026 – 05:37 pm BST

PDB ID : 7ADB / pdb\_00007adb  
EMDB ID : EMD-11722  
Title : Transcription termination intermediate complex 1 delta NusG  
Authors : Said, N.; Hilal, T.; Loll, B.; Wahl, C.M.  
Deposited on : 2020-09-14  
Resolution : 4.40 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

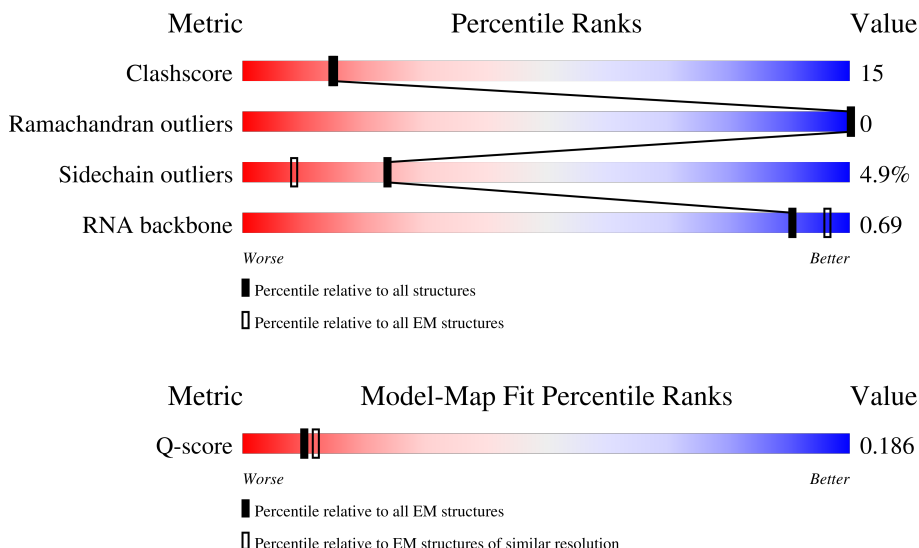
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 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                       | 3132 ( 3.91 - 4.90 )                                     |

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>74%</div> <div> <div>55%</div> <div>38%</div> <div>6%</div> </div> </div> |
| 1   | b     | 419    | <div> <div>49%</div> <div> <div>54%</div> <div>40%</div> <div>6%</div> </div> </div> |
| 1   | c     | 419    | <div> <div>45%</div> <div> <div>53%</div> <div>40%</div> <div>6%</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     |                  |

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 51330 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   | 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 |         |       |
| 1   | f     | 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     | 322      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2510  | 1569 | 442 | 491 | 8 |         |       |
| 3   | V     | 235      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1828  | 1137 | 326 | 359 | 6 |         |       |

- 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     | 24       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 497   | 235 | 95 | 143 | 24 |         |       |

- Molecule 8 is a DNA chain called tDNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 8   | L     | 34       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 682   | 325 | 122 | 202 | 33 |         |       |

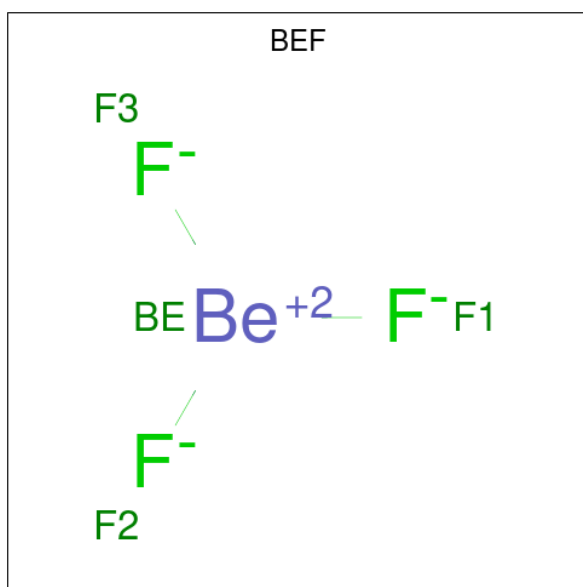
- Molecule 9 is a RNA chain called rut RNA.

| Mol | Chain | Residues | Atoms        |          |         |          |         | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|----------|---------|---------|-------|
| 9   | R     | 17       | Total<br>364 | C<br>162 | N<br>65 | O<br>120 | P<br>17 | 0       | 0     |

There are 27 discrepancies between the modelled and reference sequences:

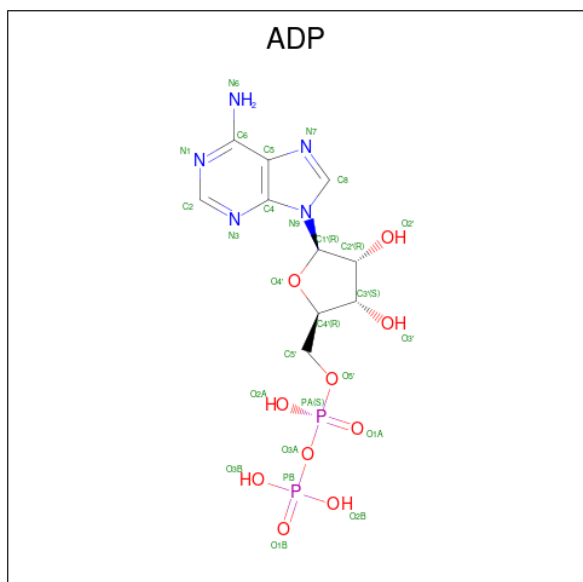
| Chain | Residue | Modelled | Actual | Comment        | Reference     |
|-------|---------|----------|--------|----------------|---------------|
| R     | 1       | G        | -      | expression tag | GB 1227111474 |
| R     | 2       | G        | -      | expression tag | GB 1227111474 |
| R     | 3       | G        | -      | expression tag | GB 1227111474 |
| R     | 72      | U        | -      | insertion      | GB 1227111474 |
| R     | 77      | U        | -      | expression tag | GB 1227111474 |
| R     | 78      | U        | -      | expression tag | GB 1227111474 |
| R     | 79      | A        | -      | expression tag | GB 1227111474 |
| R     | 80      | A        | -      | expression tag | GB 1227111474 |
| R     | 81      | A        | -      | expression tag | GB 1227111474 |
| R     | 82      | C        | -      | expression tag | GB 1227111474 |
| R     | 83      | C        | -      | expression tag | GB 1227111474 |
| R     | 84      | A        | -      | expression tag | GB 1227111474 |
| R     | 85      | C        | -      | expression tag | GB 1227111474 |
| R     | 86      | A        | -      | expression tag | GB 1227111474 |
| R     | 87      | C        | -      | expression tag | GB 1227111474 |
| R     | 88      | C        | -      | expression tag | GB 1227111474 |
| R     | 89      | U        | -      | expression tag | GB 1227111474 |
| R     | 90      | G        | -      | expression tag | GB 1227111474 |
| R     | 91      | G        | -      | expression tag | GB 1227111474 |
| R     | 92      | C        | -      | expression tag | GB 1227111474 |
| R     | 93      | G        | -      | expression tag | GB 1227111474 |
| R     | 94      | U        | -      | expression tag | GB 1227111474 |
| R     | 95      | G        | -      | expression tag | GB 1227111474 |
| R     | 96      | U        | -      | expression tag | GB 1227111474 |
| R     | 97      | G        | -      | expression tag | GB 1227111474 |
| R     | 98      | G        | -      | expression tag | GB 1227111474 |
| R     | 99      | C        | -      | expression tag | GB 1227111474 |

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 10  | b     | 1        | Total | Be | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 10  | c     | 1        | Total | Be | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 10  | d     | 1        | Total | Be | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 10  | e     | 1        | Total | Be | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 10  | f     | 1        | Total | Be | F | 0       |
|     |       |          | 4     | 1  | 3 |         |

- Molecule 11 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 |
|-----|-------|----------|-------|----|---|----|---|---------|
| 11  | b     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 11  | c     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 11  | d     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 11  | e     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 11  | f     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 12  | b     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | c     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | d     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | e     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | f     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 12  | Y     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 14 is water.

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 14  | b     | 3        | Total | O | 0       |
|     |       |          | 3     | 3 |         |
| 14  | c     | 3        | Total | O | 0       |
|     |       |          | 3     | 3 |         |
| 14  | d     | 3        | Total | O | 0       |
|     |       |          | 3     | 3 |         |

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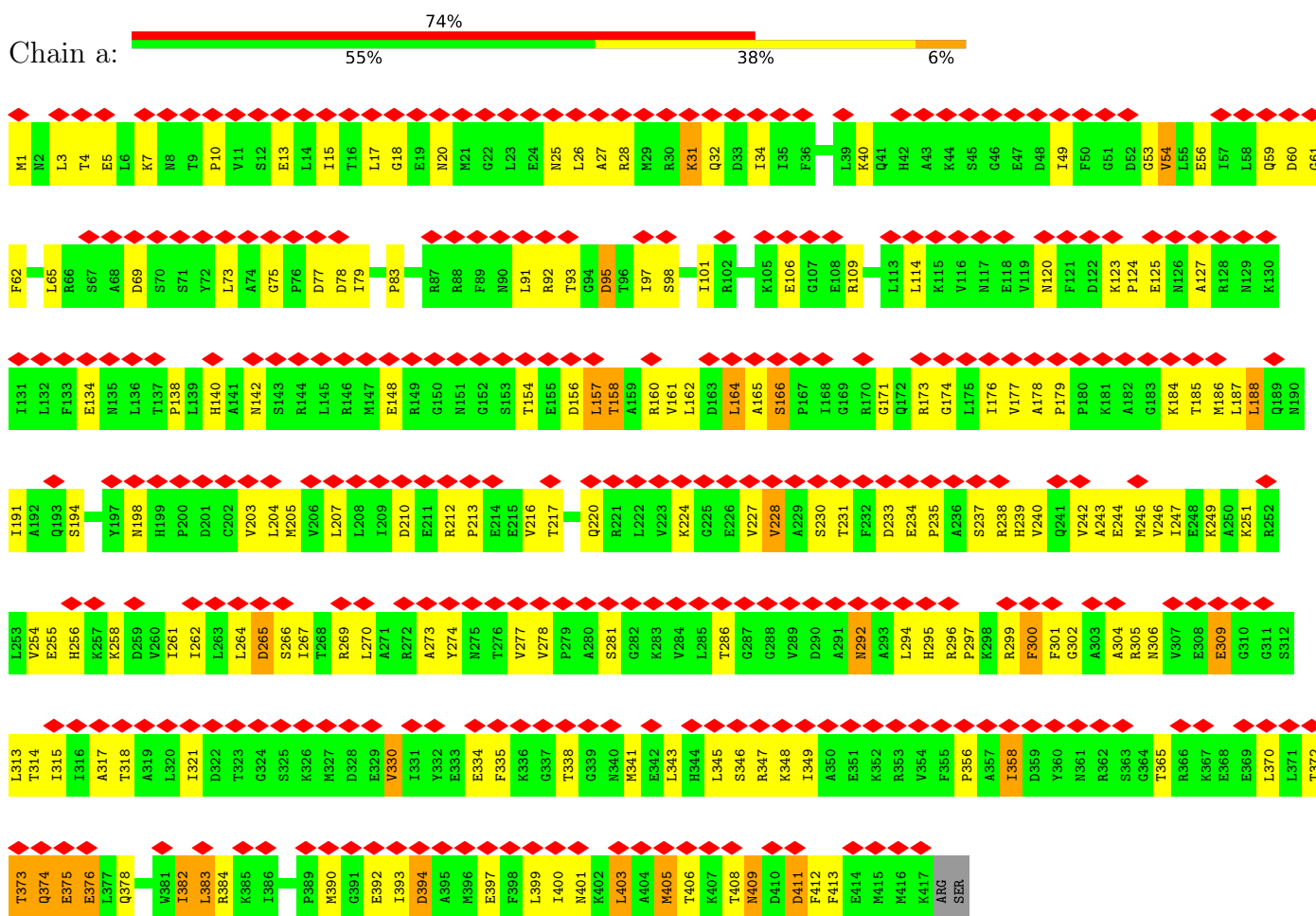
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| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 14  | e     | 3        | Total | O | 0       |
|     |       |          | 3     | 3 |         |
| 14  | f     | 3        | Total | O | 0       |
|     |       |          | 3     | 3 |         |

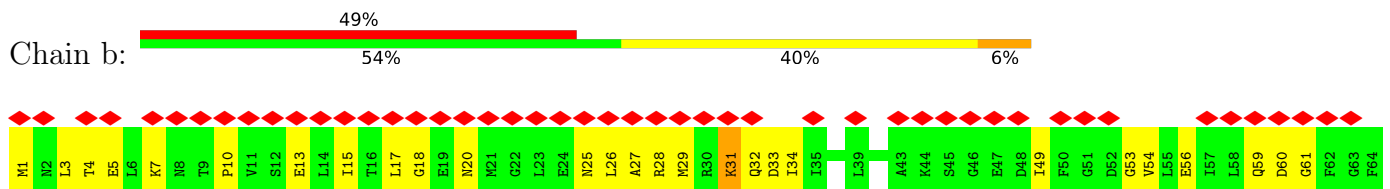
### 3 Residue-property plots

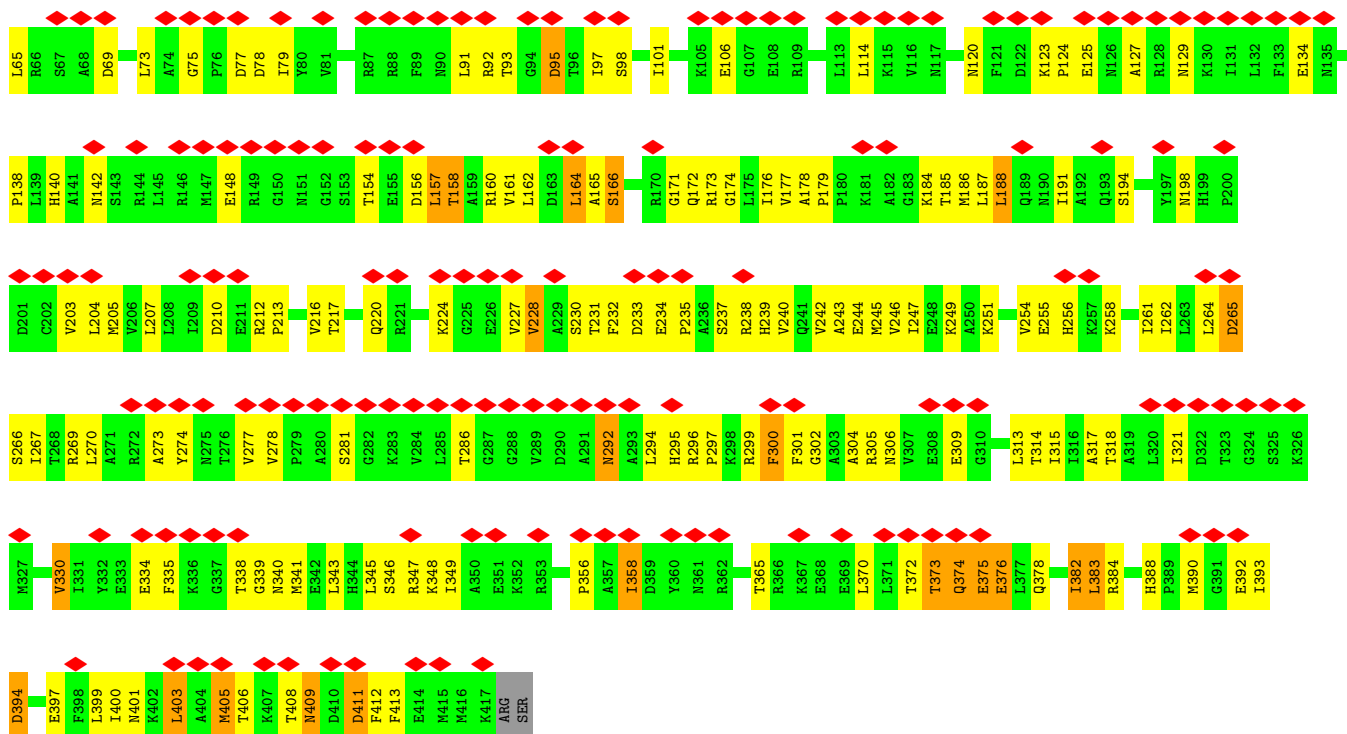
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

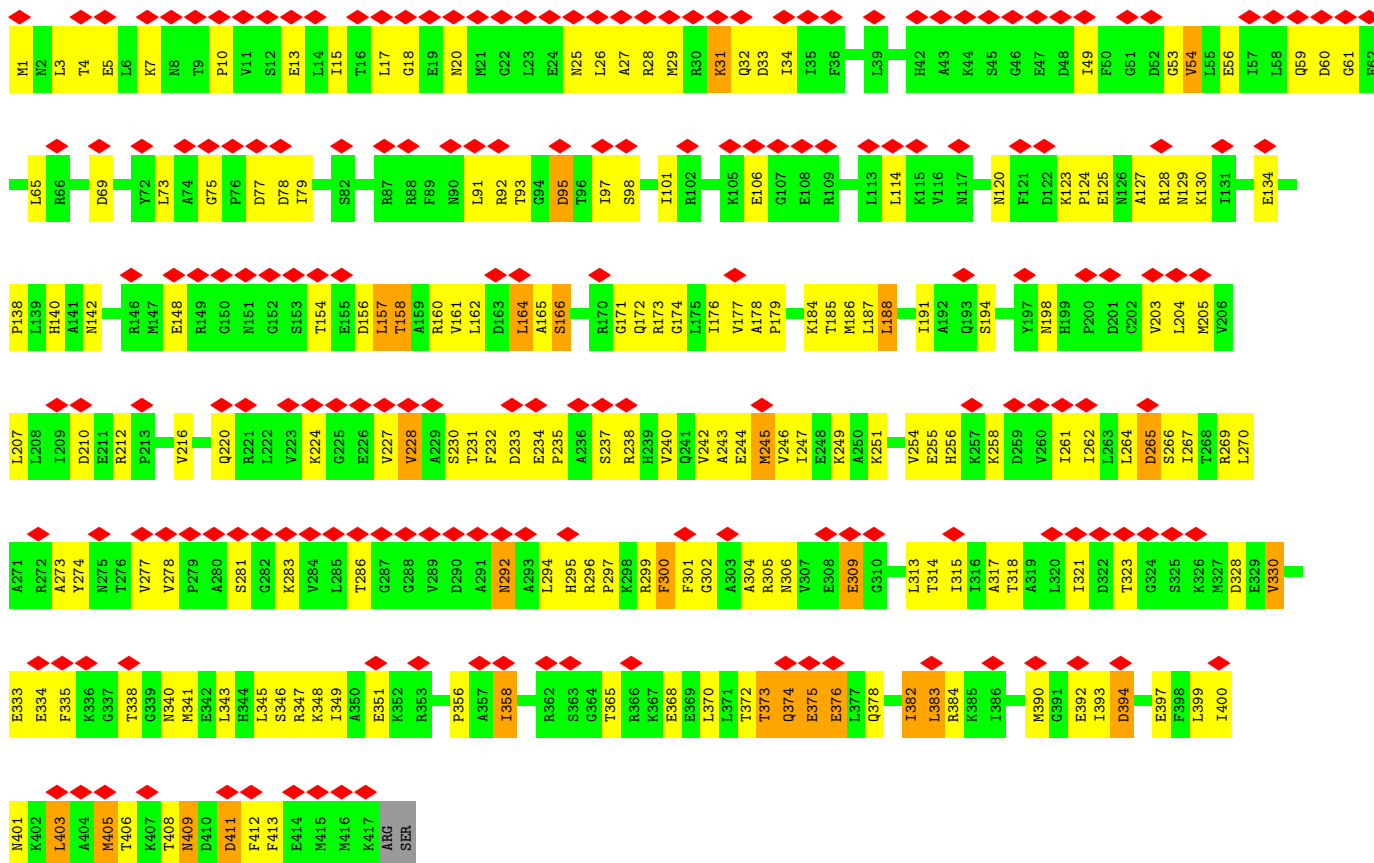
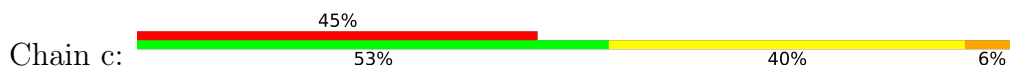


#### • Molecule 1: Transcription termination factor Rho

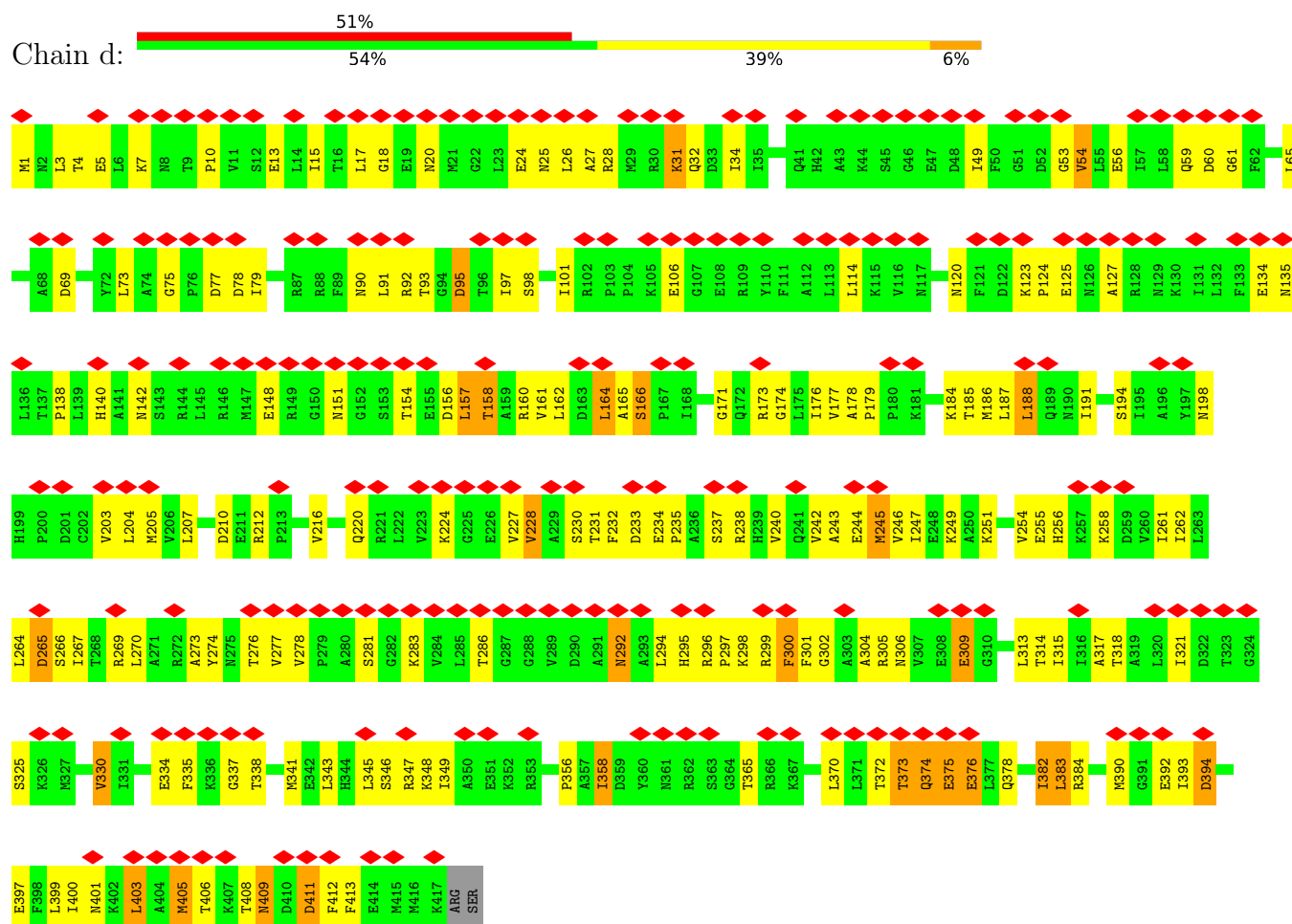




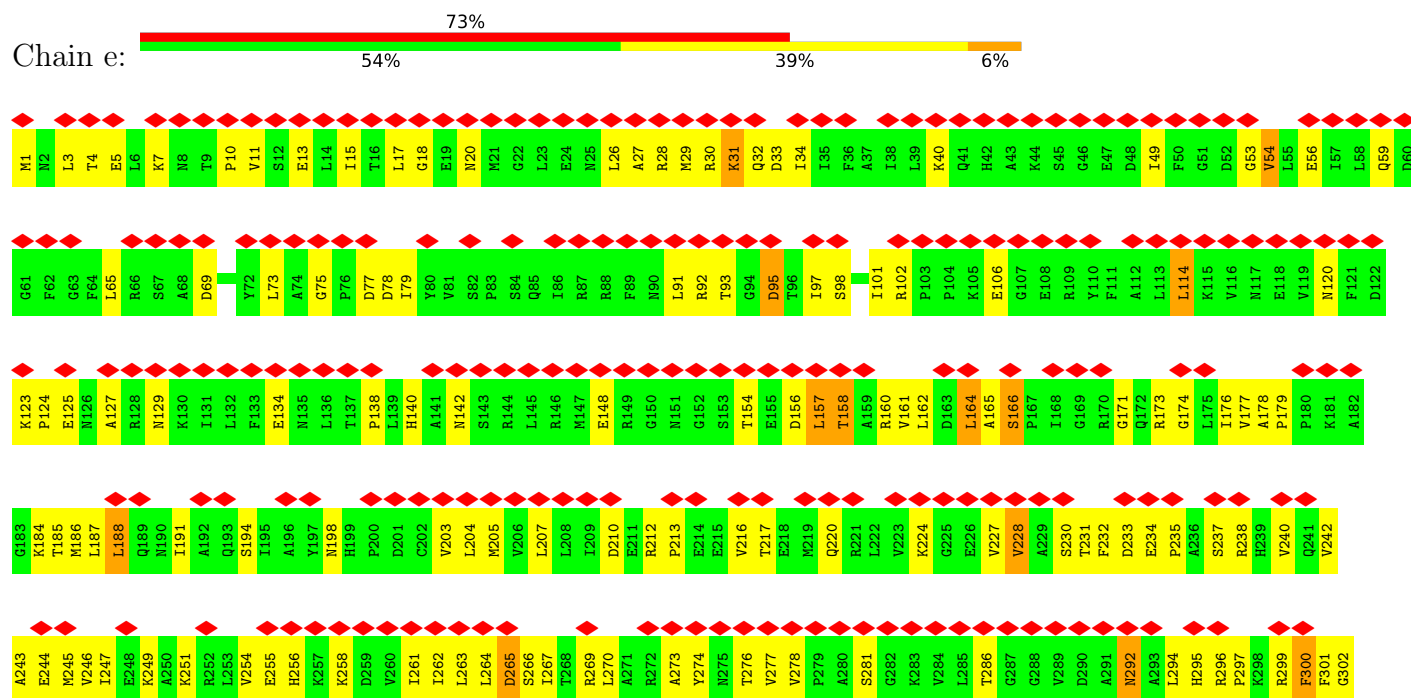
• Molecule 1: Transcription termination factor Rho

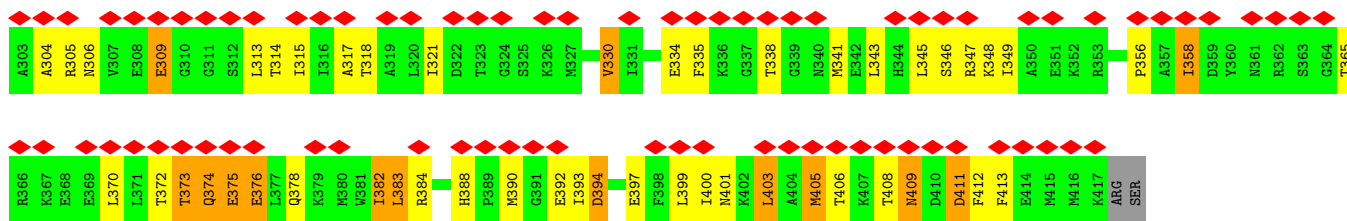


• Molecule 1: Transcription termination factor Rho

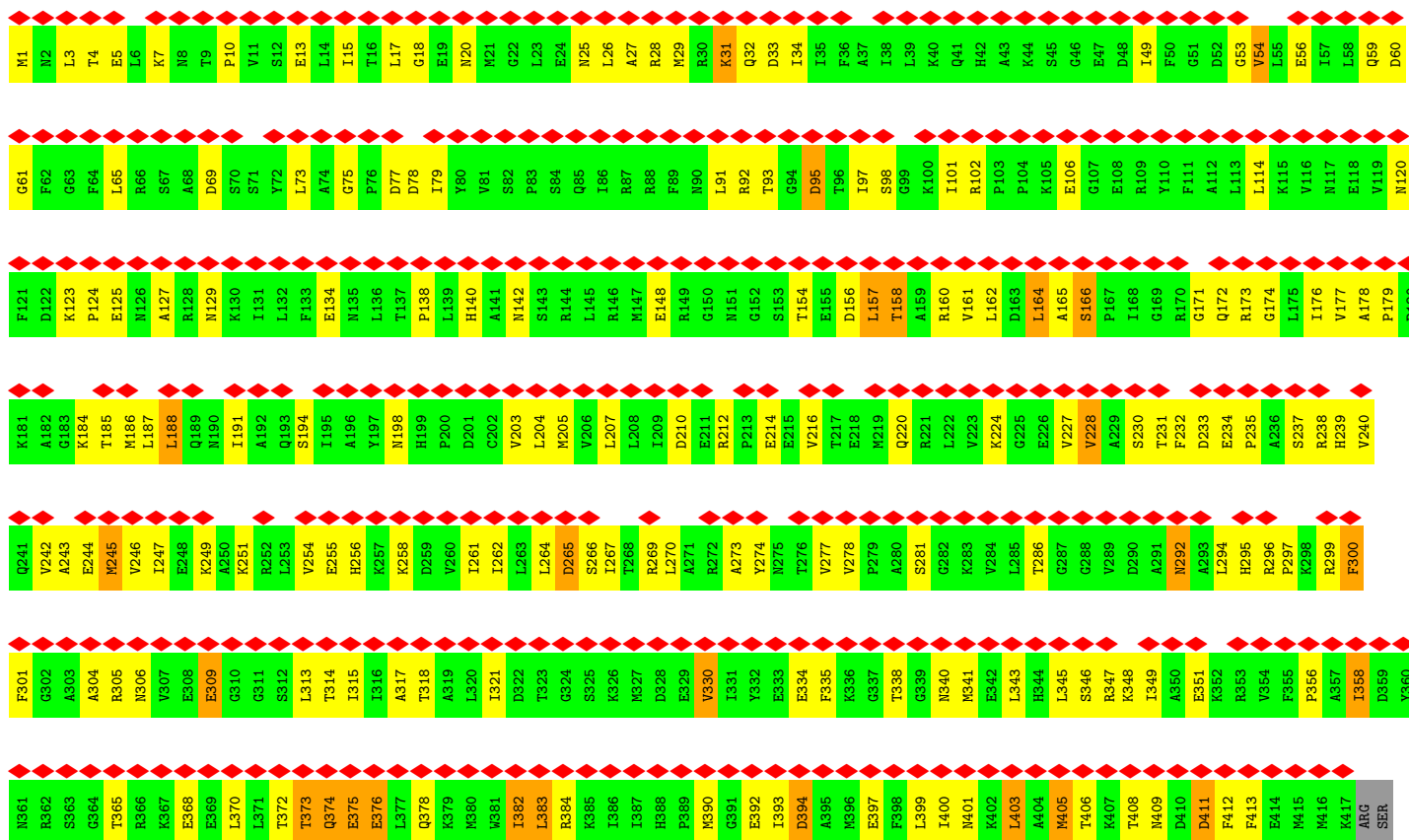


• Molecule 1: Transcription termination factor Rho



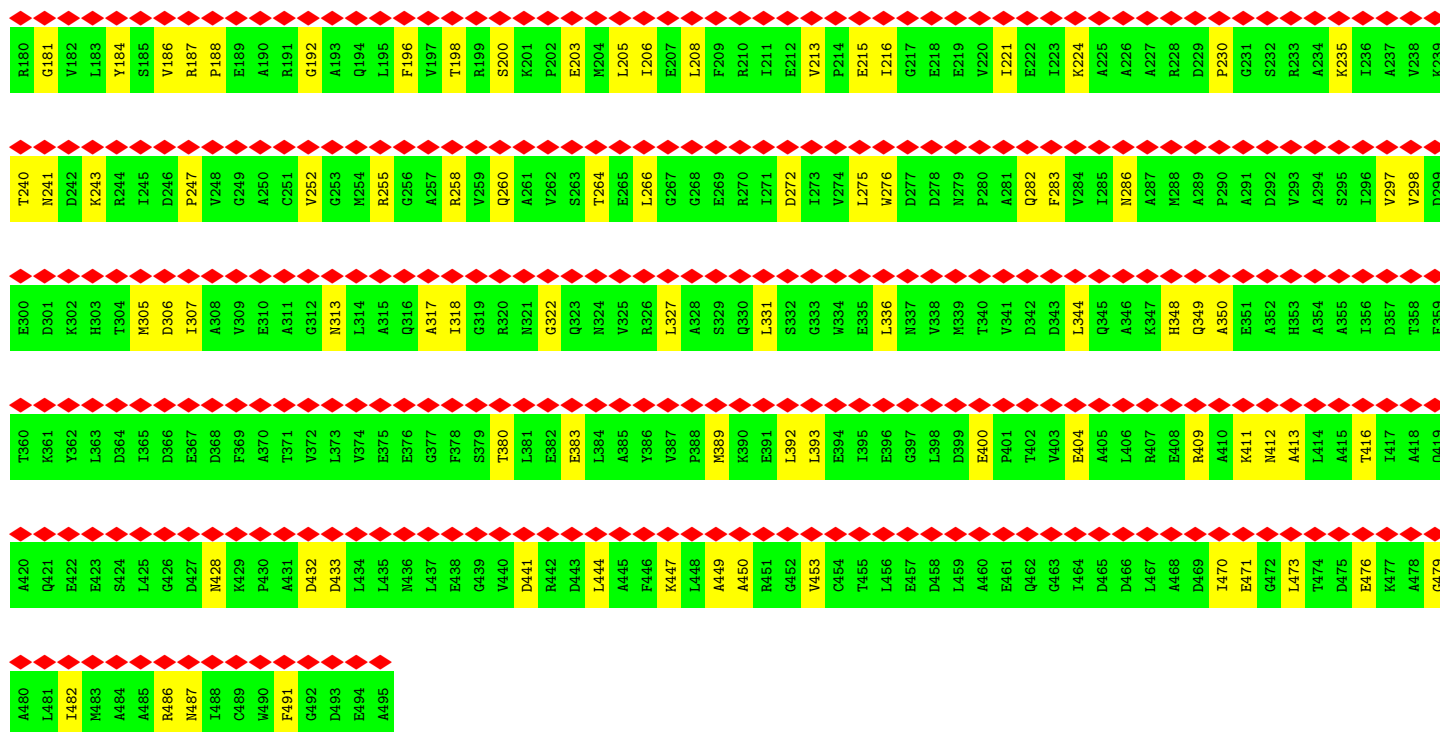


• Molecule 1: Transcription termination factor Rho

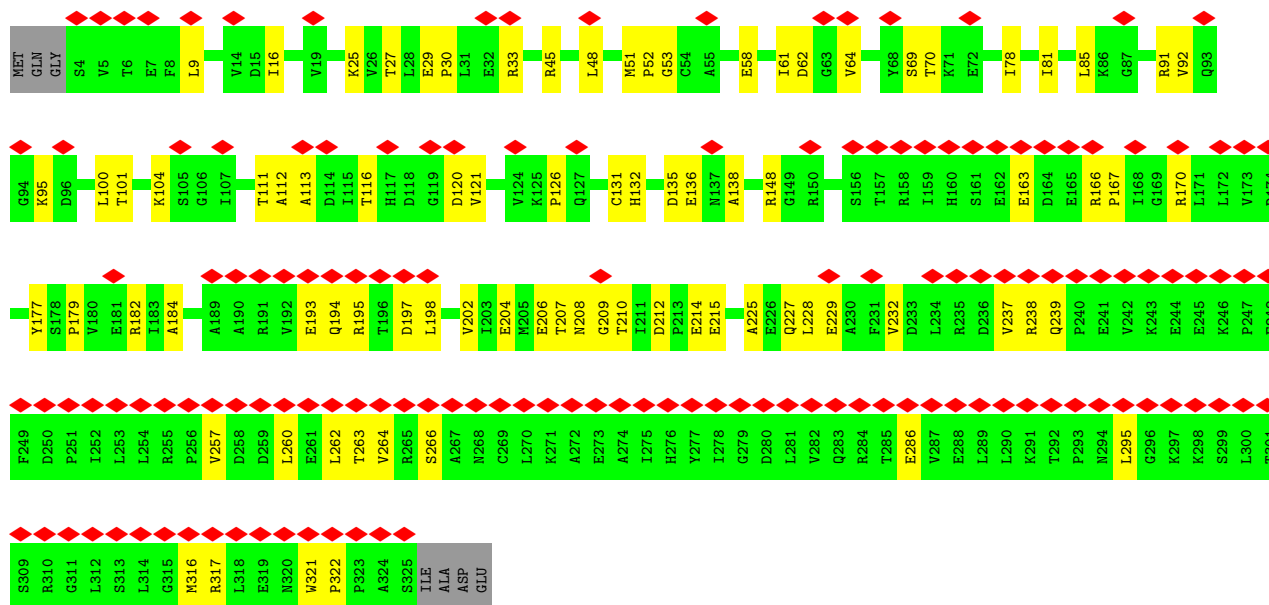
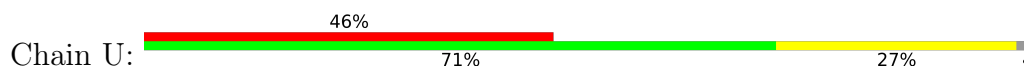


• Molecule 2: Transcription termination/antitermination protein NusA



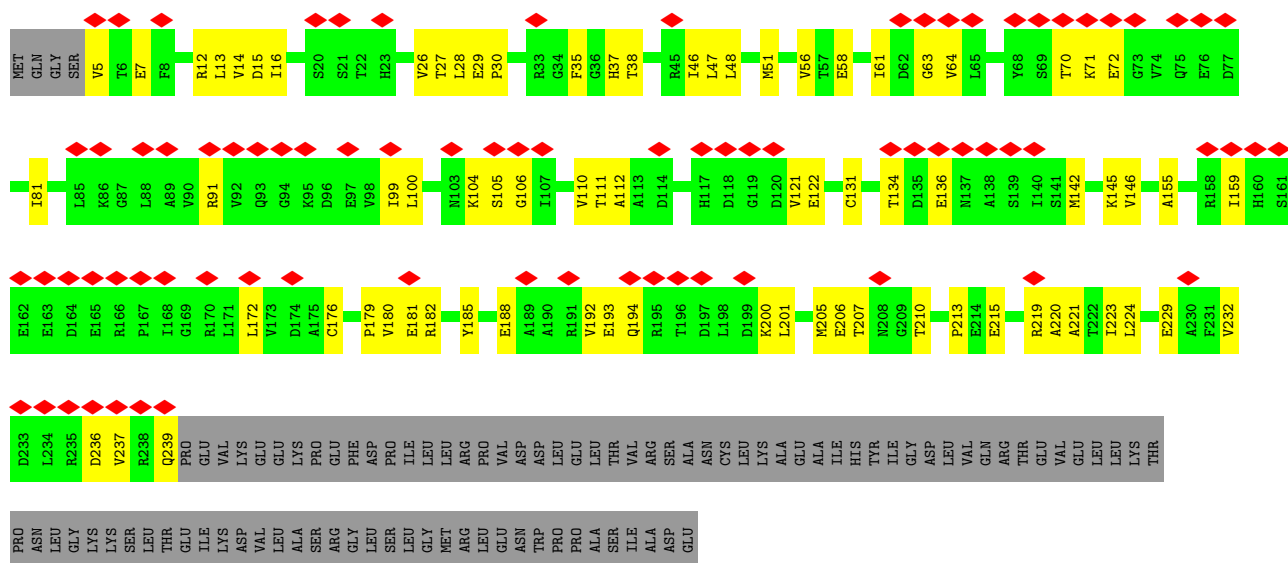


• Molecule 3: DNA-directed RNA polymerase subunit alpha

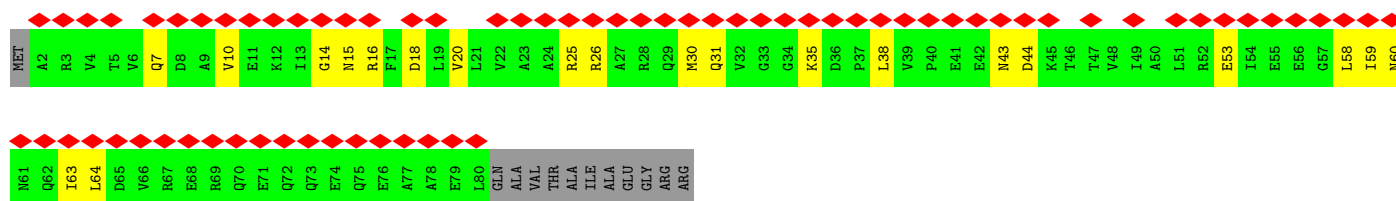
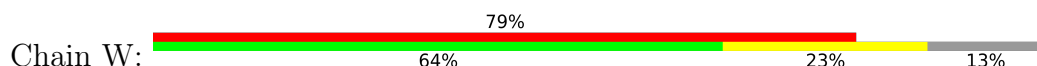


• Molecule 3: DNA-directed RNA polymerase subunit alpha

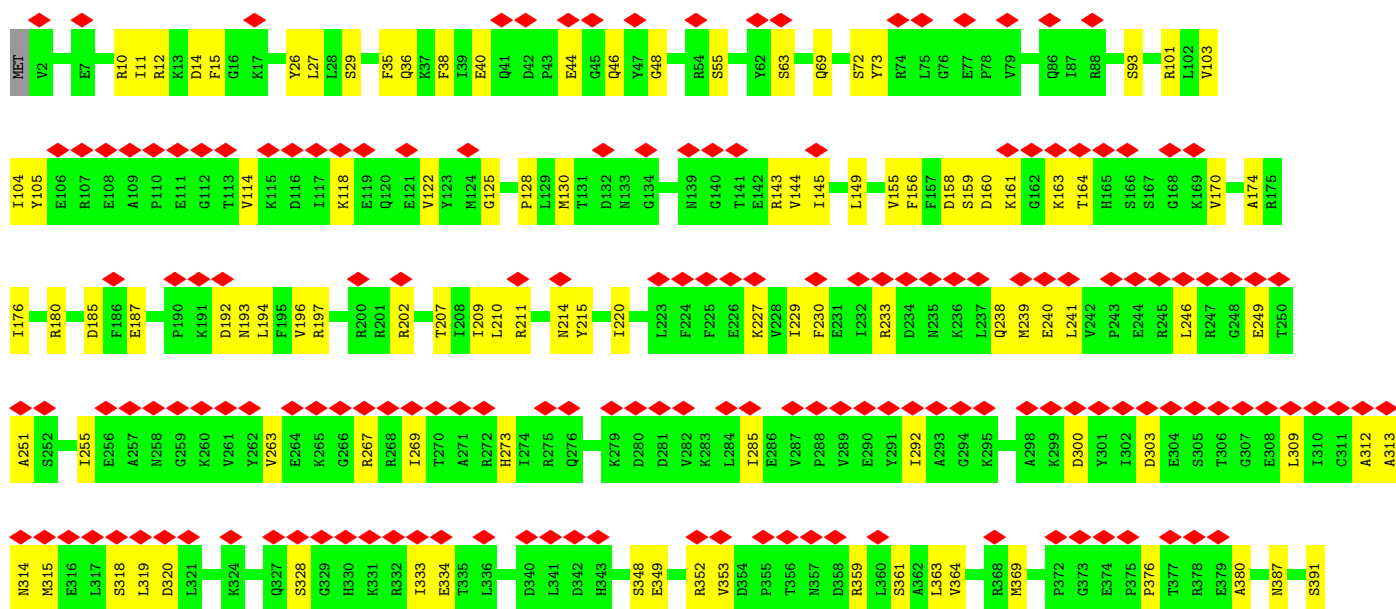


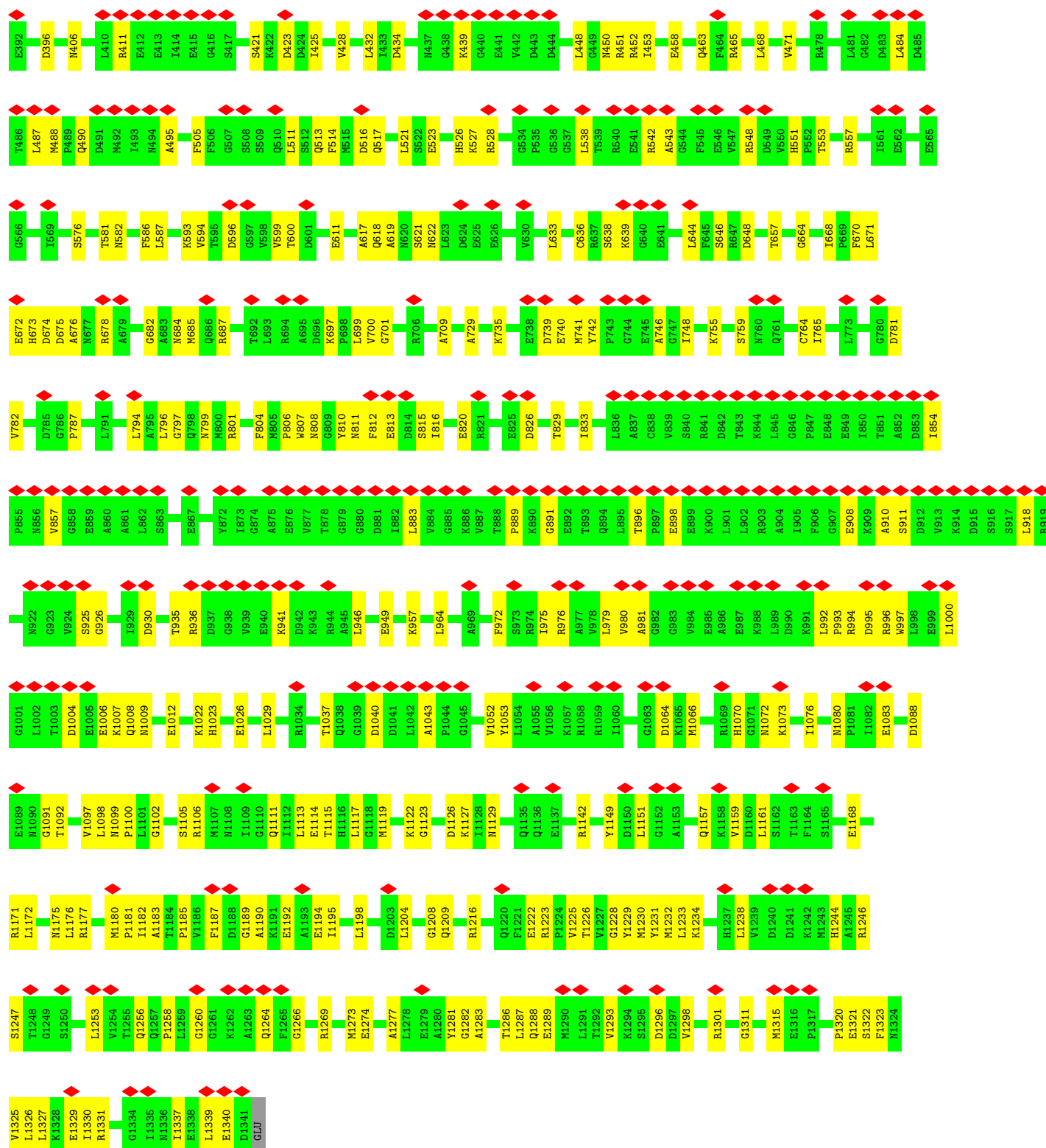


• Molecule 4: DNA-directed RNA polymerase subunit omega

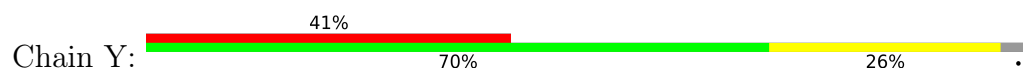


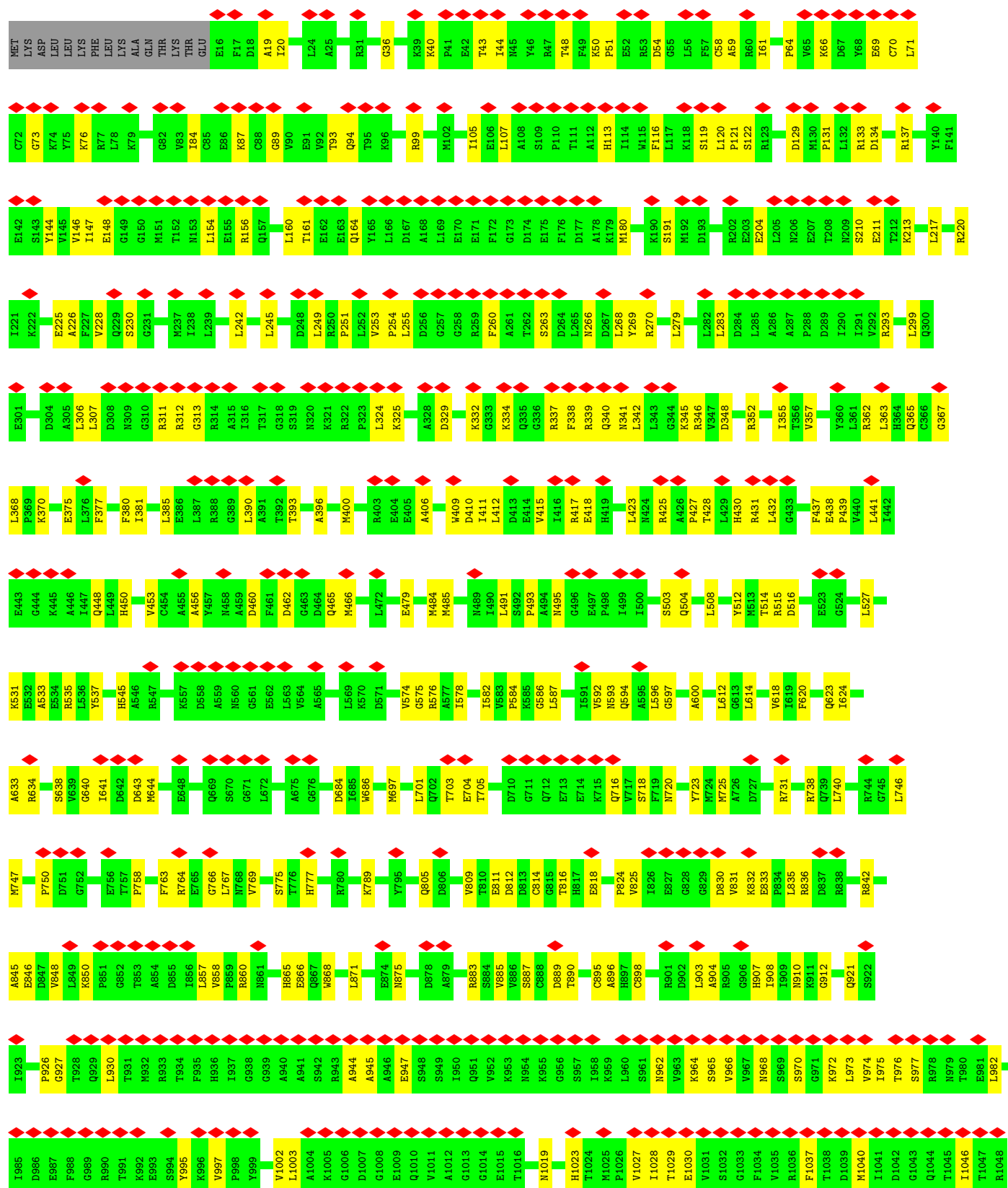
• Molecule 5: DNA-directed RNA polymerase subunit beta





- 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             | 27226                                   | 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                    | 0.247                                   | Depositor |
| Minimum map value                    | 0.000                                   | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.013                                   | 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: ADP, MG, BEF, ZN

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     | 0.17         | 0/3329      | 0.43        | 0/4483      |
| 1   | b     | 0.17         | 0/3329      | 0.43        | 0/4483      |
| 1   | c     | 0.17         | 0/3329      | 0.43        | 0/4483      |
| 1   | d     | 0.17         | 0/3329      | 0.43        | 0/4483      |
| 1   | e     | 0.17         | 0/3329      | 0.43        | 0/4483      |
| 1   | f     | 0.17         | 0/3329      | 0.43        | 0/4483      |
| 2   | A     | 0.13         | 0/3897      | 0.38        | 0/5273      |
| 3   | U     | 0.12         | 0/2544      | 0.33        | 0/3449      |
| 3   | V     | 0.12         | 0/1850      | 0.34        | 0/2507      |
| 4   | W     | 0.10         | 0/629       | 0.31        | 0/847       |
| 5   | X     | 0.11         | 0/10736     | 0.30        | 0/14487     |
| 6   | Y     | 0.10         | 0/10706     | 0.29        | 0/14456     |
| 7   | K     | 0.18         | 0/557       | 0.40        | 0/856       |
| 8   | L     | 0.18         | 0/762       | 0.36        | 0/1171      |
| 9   | R     | 0.10         | 0/405       | 0.20        | 0/627       |
| All | All   | 0.14         | 0/52060     | 0.36        | 0/70571     |

There are no bond length outliers.

There are no bond angle outliers.

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        | 3359     | 131     | 0            |
| 1   | b     | 3280  | 0        | 3357     | 134     | 0            |
| 1   | c     | 3280  | 0        | 3358     | 144     | 0            |
| 1   | d     | 3280  | 0        | 3358     | 149     | 0            |
| 1   | e     | 3280  | 0        | 3359     | 145     | 0            |
| 1   | f     | 3280  | 0        | 3358     | 134     | 0            |
| 2   | A     | 3852  | 0        | 3835     | 120     | 0            |
| 3   | U     | 2510  | 0        | 2563     | 62      | 0            |
| 3   | V     | 1828  | 0        | 1856     | 54      | 0            |
| 4   | W     | 627   | 0        | 634      | 17      | 0            |
| 5   | X     | 10567 | 0        | 10585    | 267     | 0            |
| 6   | Y     | 10545 | 0        | 10760    | 252     | 0            |
| 7   | K     | 497   | 0        | 271      | 14      | 0            |
| 8   | L     | 682   | 0        | 382      | 16      | 0            |
| 9   | R     | 364   | 0        | 184      | 8       | 0            |
| 10  | b     | 4     | 0        | 0        | 0       | 0            |
| 10  | c     | 4     | 0        | 0        | 0       | 0            |
| 10  | d     | 4     | 0        | 0        | 1       | 0            |
| 10  | e     | 4     | 0        | 0        | 1       | 0            |
| 10  | f     | 4     | 0        | 0        | 0       | 0            |
| 11  | b     | 27    | 0        | 12       | 2       | 0            |
| 11  | c     | 27    | 0        | 12       | 0       | 0            |
| 11  | d     | 27    | 0        | 12       | 1       | 0            |
| 11  | e     | 27    | 0        | 12       | 1       | 0            |
| 11  | f     | 27    | 0        | 12       | 1       | 0            |
| 12  | Y     | 1     | 0        | 0        | 0       | 0            |
| 12  | b     | 1     | 0        | 0        | 0       | 0            |
| 12  | c     | 1     | 0        | 0        | 0       | 0            |
| 12  | d     | 1     | 0        | 0        | 0       | 0            |
| 12  | e     | 1     | 0        | 0        | 0       | 0            |
| 12  | f     | 1     | 0        | 0        | 0       | 0            |
| 13  | Y     | 2     | 0        | 0        | 0       | 0            |
| 14  | b     | 3     | 0        | 0        | 0       | 0            |
| 14  | c     | 3     | 0        | 0        | 0       | 0            |
| 14  | d     | 3     | 0        | 0        | 0       | 0            |
| 14  | e     | 3     | 0        | 0        | 0       | 0            |
| 14  | f     | 3     | 0        | 0        | 0       | 0            |
| All | All   | 51330 | 0        | 51279    | 1542    | 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 15.

All (1542) 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:c:128:ARG:O     | 1:d:28:ARG:NH1    | 2.10                     | 0.85              |
| 1:d:135:ASN:HB3   | 1:e:11:VAL:HG11   | 1.60                     | 0.83              |
| 5:X:994:ARG:HA    | 5:X:997:TRP:HB2   | 1.60                     | 0.82              |
| 6:Y:703:THR:HG22  | 6:Y:704:GLU:H     | 1.46                     | 0.80              |
| 1:b:302:GLY:HA3   | 1:c:232:PHE:CZ    | 2.18                     | 0.79              |
| 6:Y:362:ARG:H     | 6:Y:365:GLN:HE21  | 1.29                     | 0.78              |
| 6:Y:926:PRO:HG2   | 6:Y:1248:ILE:HD11 | 1.66                     | 0.77              |
| 6:Y:432:LEU:HD21  | 6:Y:456:ALA:HB1   | 1.67                     | 0.76              |
| 5:X:1129:ASN:HB3  | 5:X:1177:ARG:HG3  | 1.67                     | 0.75              |
| 5:X:517:GLN:HB3   | 5:X:759:SER:HB2   | 1.69                     | 0.75              |
| 1:a:59:GLN:HG3    | 7:K:-18:DC:H5'    | 1.67                     | 0.75              |
| 6:Y:268:LEU:HD11  | 6:Y:324:LEU:HB3   | 1.71                     | 0.73              |
| 1:d:160:ARG:HH12  | 1:d:406:THR:HG23  | 1.54                     | 0.72              |
| 2:A:164:ARG:HA    | 2:A:167:MET:HE2   | 1.71                     | 0.72              |
| 1:e:160:ARG:HH12  | 1:e:406:THR:HG23  | 1.54                     | 0.72              |
| 6:Y:44:ILE:HG22   | 6:Y:51:PRO:HA     | 1.71                     | 0.72              |
| 1:c:297:PRO:HB2   | 1:c:335:PHE:HZ    | 1.55                     | 0.72              |
| 1:b:297:PRO:HB2   | 1:b:335:PHE:HZ    | 1.55                     | 0.72              |
| 1:f:160:ARG:HH12  | 1:f:406:THR:HG23  | 1.54                     | 0.72              |
| 4:W:53:GLU:HB3    | 4:W:59:ILE:HD13   | 1.70                     | 0.72              |
| 6:Y:809:VAL:HG13  | 6:Y:912:GLY:H     | 1.54                     | 0.72              |
| 1:a:160:ARG:HH12  | 1:a:406:THR:HG23  | 1.54                     | 0.72              |
| 1:f:297:PRO:HB2   | 1:f:335:PHE:HZ    | 1.55                     | 0.72              |
| 2:A:26:ALA:HB2    | 2:A:117:LYS:HD3   | 1.70                     | 0.72              |
| 1:b:160:ARG:HH12  | 1:b:406:THR:HG23  | 1.54                     | 0.71              |
| 1:c:160:ARG:HH12  | 1:c:406:THR:HG23  | 1.54                     | 0.71              |
| 5:X:180:ARG:HB3   | 5:X:396:ASP:HB2   | 1.73                     | 0.71              |
| 6:Y:245:LEU:HD21  | 6:Y:249:LEU:HB2   | 1.72                     | 0.71              |
| 5:X:207:THR:HB    | 5:X:211:ARG:HH21  | 1.55                     | 0.71              |
| 9:R:90:G:H4'      | 9:R:91:G:H5'      | 1.71                     | 0.71              |
| 1:b:302:GLY:HA3   | 1:c:232:PHE:CE1   | 2.26                     | 0.71              |
| 1:d:297:PRO:HB2   | 1:d:335:PHE:HZ    | 1.55                     | 0.71              |
| 4:W:10:VAL:HG11   | 4:W:16:ARG:HG3    | 1.72                     | 0.70              |
| 6:Y:1307:LEU:HD13 | 6:Y:1311:LYS:HB2  | 1.72                     | 0.70              |
| 1:e:297:PRO:HB2   | 1:e:335:PHE:HZ    | 1.55                     | 0.70              |
| 1:e:373:THR:OG1   | 1:e:374:GLN:N     | 2.23                     | 0.70              |
| 6:Y:885:VAL:HG11  | 6:Y:1255:VAL:HG23 | 1.71                     | 0.70              |
| 1:b:210:ASP:HB2   | 1:b:269:ARG:HD3   | 1.74                     | 0.70              |
| 1:a:297:PRO:HB2   | 1:a:335:PHE:HZ    | 1.55                     | 0.70              |
| 1:a:373:THR:OG1   | 1:a:374:GLN:N     | 2.23                     | 0.70              |
| 1:b:373:THR:OG1   | 1:b:374:GLN:N     | 2.23                     | 0.70              |
| 6:Y:120:LEU:HB3   | 6:Y:1330:ARG:HH21 | 1.55                     | 0.70              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:X:672:GLU:HB2   | 6:Y:767:LEU:HB2  | 1.73                     | 0.70              |
| 5:X:1072:ASN:HD21 | 5:X:1230:MET:HE1 | 1.55                     | 0.70              |
| 1:b:148:GLU:O     | 1:b:198:ASN:ND2  | 2.25                     | 0.70              |
| 1:c:148:GLU:O     | 1:c:198:ASN:ND2  | 2.25                     | 0.70              |
| 1:c:210:ASP:HB2   | 1:c:269:ARG:HD3  | 1.74                     | 0.70              |
| 1:e:210:ASP:HB2   | 1:e:269:ARG:HD3  | 1.74                     | 0.70              |
| 5:X:1073:LYS:HD2  | 6:Y:462:ASP:HB2  | 1.74                     | 0.70              |
| 1:e:148:GLU:O     | 1:e:198:ASN:ND2  | 2.25                     | 0.69              |
| 1:d:148:GLU:O     | 1:d:198:ASN:ND2  | 2.25                     | 0.69              |
| 1:d:210:ASP:HB2   | 1:d:269:ARG:HD3  | 1.74                     | 0.69              |
| 1:f:210:ASP:HB2   | 1:f:269:ARG:HD3  | 1.74                     | 0.69              |
| 6:Y:582:ILE:HD12  | 6:Y:623:GLN:HB3  | 1.75                     | 0.69              |
| 1:b:165:ALA:O     | 1:b:384:ARG:NH2  | 2.26                     | 0.69              |
| 1:c:165:ALA:O     | 1:c:384:ARG:NH2  | 2.26                     | 0.69              |
| 1:f:148:GLU:O     | 1:f:198:ASN:ND2  | 2.25                     | 0.69              |
| 1:a:148:GLU:O     | 1:a:198:ASN:ND2  | 2.25                     | 0.69              |
| 1:e:165:ALA:O     | 1:e:384:ARG:NH2  | 2.26                     | 0.69              |
| 5:X:12:ARG:HD3    | 5:X:1183:ALA:HB2 | 1.75                     | 0.69              |
| 6:Y:425:ARG:HG3   | 6:Y:427:PRO:HD2  | 1.75                     | 0.69              |
| 6:Y:584:PRO:HG2   | 6:Y:587:LEU:HD23 | 1.73                     | 0.69              |
| 3:V:58:GLU:HB3    | 3:V:145:LYS:HB3  | 1.73                     | 0.69              |
| 1:d:165:ALA:O     | 1:d:384:ARG:NH2  | 2.26                     | 0.69              |
| 1:a:165:ALA:O     | 1:a:384:ARG:NH2  | 2.26                     | 0.69              |
| 1:c:254:VAL:HG21  | 1:c:313:LEU:HB2  | 1.76                     | 0.68              |
| 1:c:302:GLY:HA3   | 1:d:232:PHE:CZ   | 2.28                     | 0.68              |
| 4:W:26:ARG:HH22   | 4:W:35:LYS:HD2   | 1.58                     | 0.68              |
| 5:X:1298:VAL:HA   | 5:X:1301:ARG:HE  | 1.57                     | 0.68              |
| 1:d:254:VAL:HG21  | 1:d:313:LEU:HB2  | 1.76                     | 0.68              |
| 1:a:210:ASP:HB2   | 1:a:269:ARG:HD3  | 1.74                     | 0.68              |
| 1:f:53:GLY:HA3    | 1:f:65:LEU:HB3   | 1.76                     | 0.68              |
| 5:X:269:ILE:HG23  | 5:X:273:HIS:HB2  | 1.76                     | 0.68              |
| 2:A:205:LEU:HA    | 2:A:208:LEU:HD12 | 1.75                     | 0.68              |
| 3:V:176:CYS:SG    | 6:Y:535:ARG:NH2  | 2.62                     | 0.68              |
| 1:c:53:GLY:HA3    | 1:c:65:LEU:HB3   | 1.76                     | 0.68              |
| 1:d:138:PRO:HD2   | 1:e:217:THR:HG21 | 1.76                     | 0.68              |
| 1:e:53:GLY:HA3    | 1:e:65:LEU:HB3   | 1.76                     | 0.68              |
| 1:a:53:GLY:HA3    | 1:a:65:LEU:HB3   | 1.76                     | 0.68              |
| 1:f:165:ALA:O     | 1:f:384:ARG:NH2  | 2.26                     | 0.68              |
| 1:f:254:VAL:HG21  | 1:f:313:LEU:HB2  | 1.76                     | 0.68              |
| 1:b:53:GLY:HA3    | 1:b:65:LEU:HB3   | 1.76                     | 0.68              |
| 1:f:203:VAL:HG21  | 1:f:258:LYS:HE2  | 1.76                     | 0.68              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:U:135:ASP:HB3   | 3:U:138:ALA:HB2  | 1.76                     | 0.68              |
| 6:Y:842:ARG:HD3   | 6:Y:1251:LYS:HZ2 | 1.57                     | 0.68              |
| 6:Y:64:PRO:HG2    | 6:Y:93:THR:H     | 1.58                     | 0.68              |
| 1:a:203:VAL:HG21  | 1:a:258:LYS:HE2  | 1.76                     | 0.67              |
| 1:a:254:VAL:HG21  | 1:a:313:LEU:HB2  | 1.76                     | 0.67              |
| 1:e:254:VAL:HG21  | 1:e:313:LEU:HB2  | 1.76                     | 0.67              |
| 1:d:53:GLY:HA3    | 1:d:65:LEU:HB3   | 1.76                     | 0.67              |
| 5:X:1246:ARG:HH11 | 5:X:1266:GLY:HA2 | 1.60                     | 0.67              |
| 1:b:254:VAL:HG21  | 1:b:313:LEU:HB2  | 1.76                     | 0.67              |
| 1:d:90:ASN:CB     | 1:e:28:ARG:HD3   | 2.25                     | 0.67              |
| 1:f:375:GLU:OE2   | 1:f:376:GLU:N    | 2.28                     | 0.67              |
| 2:A:19:PRO:HD2    | 2:A:22:LYS:HE2   | 1.75                     | 0.67              |
| 1:a:375:GLU:OE2   | 1:a:376:GLU:N    | 2.28                     | 0.67              |
| 1:c:203:VAL:HG21  | 1:c:258:LYS:HE2  | 1.76                     | 0.66              |
| 1:b:203:VAL:HG21  | 1:b:258:LYS:HE2  | 1.76                     | 0.66              |
| 1:e:203:VAL:HG21  | 1:e:258:LYS:HE2  | 1.76                     | 0.66              |
| 1:b:375:GLU:OE2   | 1:b:376:GLU:N    | 2.28                     | 0.66              |
| 1:d:24:GLU:HG3    | 5:X:997:TRP:HH2  | 1.59                     | 0.66              |
| 1:c:375:GLU:OE2   | 1:c:376:GLU:N    | 2.28                     | 0.66              |
| 1:d:375:GLU:OE2   | 1:d:376:GLU:N    | 2.28                     | 0.66              |
| 1:d:203:VAL:HG21  | 1:d:258:LYS:HE2  | 1.76                     | 0.66              |
| 2:A:104:ARG:NH2   | 5:X:908:GLU:O    | 2.29                     | 0.66              |
| 5:X:312:ALA:H     | 5:X:315:MET:HE2  | 1.59                     | 0.66              |
| 5:X:804:PHE:HB3   | 5:X:1100:PRO:HB3 | 1.76                     | 0.66              |
| 1:c:373:THR:OG1   | 1:c:374:GLN:N    | 2.23                     | 0.66              |
| 5:X:26:TYR:HB3    | 5:X:29:SER:HB3   | 1.78                     | 0.66              |
| 6:Y:1223:LEU:HD12 | 6:Y:1224:ARG:HG3 | 1.78                     | 0.65              |
| 3:V:100:LEU:HD21  | 3:V:121:VAL:HG21 | 1.78                     | 0.65              |
| 5:X:729:ALA:O     | 5:X:755:LYS:NZ   | 2.29                     | 0.65              |
| 2:A:71:PRO:HG3    | 3:U:308:ALA:HB3  | 1.77                     | 0.65              |
| 3:V:56:VAL:HA     | 3:V:146:VAL:HG12 | 1.78                     | 0.65              |
| 6:Y:1295:ASN:HB2  | 6:Y:1297:LYS:HZ2 | 1.61                     | 0.65              |
| 1:e:375:GLU:OE2   | 1:e:376:GLU:N    | 2.28                     | 0.65              |
| 1:d:304:ALA:HA    | 1:d:313:LEU:HD22 | 1.79                     | 0.65              |
| 2:A:49:ILE:HA     | 2:A:56:PHE:HA    | 1.79                     | 0.65              |
| 1:e:304:ALA:HA    | 1:e:313:LEU:HD22 | 1.79                     | 0.64              |
| 5:X:1289:GLU:HG3  | 5:X:1315:MET:HE2 | 1.78                     | 0.64              |
| 3:U:212:ASP:HB3   | 3:U:215:GLU:HB3  | 1.78                     | 0.64              |
| 4:W:15:ASN:O      | 6:Y:910:ASN:ND2  | 2.29                     | 0.64              |
| 2:A:21:GLU:HA     | 2:A:24:PHE:CE2   | 2.33                     | 0.64              |
| 6:Y:36:GLY:HA3    | 6:Y:61:ILE:HG12  | 1.80                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:A:318:ILE:HG22 | 2:A:322:GLY:HA2   | 1.80                     | 0.64              |
| 3:V:16:ILE:HG23  | 3:V:26:VAL:HG12   | 1.80                     | 0.64              |
| 1:b:304:ALA:HA   | 1:b:313:LEU:HD22  | 1.79                     | 0.64              |
| 3:V:51:MET:HG3   | 3:V:179:PRO:HD2   | 1.79                     | 0.64              |
| 5:X:1273:MET:HB3 | 6:Y:428:THR:HB    | 1.79                     | 0.64              |
| 1:f:304:ALA:HA   | 1:f:313:LEU:HD22  | 1.79                     | 0.63              |
| 1:f:373:THR:OG1  | 1:f:374:GLN:N     | 2.23                     | 0.63              |
| 5:X:528:ARG:NH2  | 5:X:576:SER:O     | 2.30                     | 0.63              |
| 6:Y:824:PRO:HD3  | 6:Y:835:LEU:HD12  | 1.78                     | 0.63              |
| 1:a:304:ALA:HA   | 1:a:313:LEU:HD22  | 1.79                     | 0.63              |
| 5:X:993:PRO:O    | 5:X:997:TRP:HD1   | 1.81                     | 0.63              |
| 6:Y:846:GLU:HA   | 6:Y:860:ARG:HE    | 1.63                     | 0.63              |
| 1:c:130:LYS:H    | 1:d:28:ARG:HH22   | 1.47                     | 0.63              |
| 1:c:304:ALA:HA   | 1:c:313:LEU:HD22  | 1.79                     | 0.63              |
| 5:X:796:LEU:HB3  | 5:X:1233:LEU:HD21 | 1.79                     | 0.63              |
| 6:Y:586:GLY:HA3  | 6:Y:612:LEU:HD21  | 1.81                     | 0.63              |
| 7:K:4:DG:H2'     | 7:K:5:DA:C8       | 2.33                     | 0.63              |
| 1:f:140:HIS:O    | 1:f:306:ASN:ND2   | 2.26                     | 0.63              |
| 2:A:142:VAL:HG23 | 2:A:175:PRO:HA    | 1.81                     | 0.63              |
| 5:X:103:VAL:HB   | 5:X:114:VAL:HG21  | 1.80                     | 0.63              |
| 2:A:297:VAL:HB   | 2:A:306:ASP:HB3   | 1.81                     | 0.62              |
| 4:W:14:GLY:O     | 4:W:15:ASN:ND2    | 2.33                     | 0.62              |
| 6:Y:270:ARG:HD2  | 7:K:-15:DG:H5''   | 1.81                     | 0.62              |
| 1:a:274:TYR:O    | 1:a:278:VAL:HG12  | 2.00                     | 0.62              |
| 1:c:274:TYR:O    | 1:c:278:VAL:HG12  | 1.99                     | 0.62              |
| 1:f:274:TYR:O    | 1:f:278:VAL:HG12  | 2.00                     | 0.62              |
| 3:U:58:GLU:OE1   | 3:U:170:ARG:NH2   | 2.32                     | 0.62              |
| 1:f:247:ILE:HB   | 1:f:300:PHE:CE1   | 2.35                     | 0.62              |
| 5:X:981:ALA:HB3  | 5:X:1007:LYS:HZ1  | 1.65                     | 0.62              |
| 1:c:161:VAL:HG12 | 1:c:358:ILE:HD12  | 1.82                     | 0.62              |
| 1:e:247:ILE:HB   | 1:e:300:PHE:CE1   | 2.35                     | 0.62              |
| 6:Y:857:LEU:HG   | 6:Y:858:VAL:HG23  | 1.82                     | 0.62              |
| 1:b:247:ILE:HB   | 1:b:300:PHE:CE1   | 2.35                     | 0.62              |
| 1:c:302:GLY:HA3  | 1:d:232:PHE:CE1   | 2.35                     | 0.62              |
| 6:Y:1207:GLY:HA2 | 6:Y:1223:LEU:HD13 | 1.82                     | 0.62              |
| 1:f:161:VAL:HG12 | 1:f:358:ILE:HD12  | 1.82                     | 0.62              |
| 1:f:176:ILE:HD13 | 1:f:343:LEU:HB2   | 1.81                     | 0.62              |
| 1:b:274:TYR:O    | 1:b:278:VAL:HG12  | 2.00                     | 0.61              |
| 1:d:176:ILE:HD13 | 1:d:343:LEU:HB2   | 1.81                     | 0.61              |
| 1:d:373:THR:OG1  | 1:d:374:GLN:N     | 2.23                     | 0.61              |
| 5:X:811:ASN:HB2  | 5:X:1099:ASN:HB2  | 1.82                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:d:274:TYR:O    | 1:d:278:VAL:HG12  | 1.99                     | 0.61              |
| 1:e:176:ILE:HD13 | 1:e:343:LEU:HB2   | 1.81                     | 0.61              |
| 3:V:180:VAL:HA   | 3:V:207:THR:HA    | 1.81                     | 0.61              |
| 6:Y:70:CYS:SG    | 6:Y:71:LEU:N      | 2.73                     | 0.61              |
| 6:Y:890:THR:OG1  | 6:Y:895:CYS:SG    | 2.57                     | 0.61              |
| 1:a:176:ILE:HD13 | 1:a:343:LEU:HB2   | 1.82                     | 0.61              |
| 1:e:274:TYR:O    | 1:e:278:VAL:HG12  | 2.00                     | 0.61              |
| 3:U:131:CYS:SG   | 3:U:132:HIS:N     | 2.73                     | 0.61              |
| 3:V:48:LEU:HD22  | 6:Y:535:ARG:HG3   | 1.83                     | 0.61              |
| 1:f:102:ARG:NH2  | 2:A:131:ARG:HH12  | 1.98                     | 0.61              |
| 5:X:1142:ARG:NH1 | 5:X:1161:LEU:O    | 2.34                     | 0.61              |
| 6:Y:973:LEU:HD23 | 6:Y:1003:LEU:HD23 | 1.81                     | 0.61              |
| 6:Y:982:LEU:HD23 | 6:Y:997:VAL:HG22  | 1.82                     | 0.61              |
| 1:b:388:HIS:HE1  | 1:c:351:GLU:OE1   | 1.83                     | 0.61              |
| 1:d:161:VAL:HG12 | 1:d:358:ILE:HD12  | 1.82                     | 0.61              |
| 6:Y:312:ARG:HH11 | 6:Y:313:GLY:H     | 1.48                     | 0.61              |
| 6:Y:516:ASP:HA   | 6:Y:545:HIS:HB2   | 1.82                     | 0.61              |
| 1:a:247:ILE:HB   | 1:a:300:PHE:CE1   | 2.35                     | 0.61              |
| 5:X:10:ARG:NH2   | 5:X:1175:ASN:HB3  | 2.15                     | 0.61              |
| 1:a:140:HIS:O    | 1:a:306:ASN:ND2   | 2.26                     | 0.61              |
| 1:a:349:ILE:HD11 | 1:a:392:GLU:HG3   | 1.83                     | 0.61              |
| 1:e:161:VAL:HG12 | 1:e:358:ILE:HD12  | 1.82                     | 0.61              |
| 2:A:28:GLU:OE1   | 2:A:48:GLN:N      | 2.29                     | 0.61              |
| 2:A:235:LYS:HG2  | 2:A:272:ASP:HB2   | 1.82                     | 0.61              |
| 5:X:1192:GLU:HG3 | 6:Y:641:ILE:HG12  | 1.81                     | 0.61              |
| 6:Y:225:GLU:HA   | 6:Y:228:VAL:HG22  | 1.80                     | 0.61              |
| 1:a:161:VAL:HG12 | 1:a:358:ILE:HD12  | 1.82                     | 0.61              |
| 1:b:161:VAL:HG12 | 1:b:358:ILE:HD12  | 1.82                     | 0.61              |
| 1:d:207:LEU:HD23 | 1:d:264:LEU:HD12  | 1.83                     | 0.61              |
| 1:c:207:LEU:HD23 | 1:c:264:LEU:HD12  | 1.83                     | 0.61              |
| 6:Y:903:LEU:HD21 | 6:Y:1249:ASN:HD22 | 1.66                     | 0.61              |
| 1:c:247:ILE:HB   | 1:c:300:PHE:CE1   | 2.35                     | 0.60              |
| 6:Y:833:GLU:OE1  | 6:Y:1247:LYS:NZ   | 2.33                     | 0.60              |
| 8:L:1:DT:H2'     | 8:L:2:DG:C8       | 2.35                     | 0.60              |
| 1:d:247:ILE:HB   | 1:d:300:PHE:CE1   | 2.35                     | 0.60              |
| 3:U:321:TRP:CG   | 3:U:322:PRO:HD3   | 2.37                     | 0.60              |
| 6:Y:975:ILE:HG22 | 6:Y:977:SER:H     | 1.66                     | 0.60              |
| 5:X:40:GLU:O     | 5:X:73:TYR:OH     | 2.18                     | 0.60              |
| 5:X:145:ILE:HG23 | 5:X:511:LEU:HD13  | 1.83                     | 0.60              |
| 5:X:936:ARG:NH2  | 5:X:1043:ALA:O    | 2.32                     | 0.60              |
| 1:b:207:LEU:HD23 | 1:b:264:LEU:HD12  | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:470:ILE:HG12 | 2:A:473:LEU:HB2  | 1.82                     | 0.60              |
| 3:V:5:VAL:HG23   | 3:V:7:GLU:H      | 1.66                     | 0.60              |
| 1:c:176:ILE:HD13 | 1:c:343:LEU:HB2  | 1.81                     | 0.60              |
| 2:A:31:LEU:HD22  | 2:A:47:VAL:HB    | 1.83                     | 0.60              |
| 1:b:140:HIS:O    | 1:b:306:ASN:ND2  | 2.26                     | 0.60              |
| 3:U:64:VAL:HG21  | 3:U:78:ILE:HG13  | 1.84                     | 0.60              |
| 5:X:349:GLU:HA   | 5:X:352:ARG:HG2  | 1.84                     | 0.60              |
| 5:X:1119:MET:HB2 | 5:X:1228:GLY:HA2 | 1.84                     | 0.60              |
| 1:b:176:ILE:HD13 | 1:b:343:LEU:HB2  | 1.82                     | 0.60              |
| 1:d:349:ILE:HD11 | 1:d:392:GLU:HG3  | 1.83                     | 0.60              |
| 5:X:889:PRO:HB3  | 5:X:910:ALA:HB3  | 1.83                     | 0.60              |
| 2:A:482:ILE:HG23 | 2:A:486:ARG:HH21 | 1.67                     | 0.60              |
| 5:X:156:PHE:HE2  | 5:X:450:ASN:HB3  | 1.65                     | 0.60              |
| 5:X:633:LEU:HD11 | 5:X:644:LEU:HD23 | 1.83                     | 0.60              |
| 1:a:207:LEU:HD23 | 1:a:264:LEU:HD12 | 1.83                     | 0.60              |
| 1:b:244:GLU:HA   | 1:b:247:ILE:HG22 | 1.84                     | 0.60              |
| 1:c:140:HIS:O    | 1:c:306:ASN:ND2  | 2.26                     | 0.60              |
| 1:c:349:ILE:HD11 | 1:c:392:GLU:HG3  | 1.83                     | 0.60              |
| 1:d:244:GLU:HA   | 1:d:247:ILE:HG22 | 1.84                     | 0.60              |
| 6:Y:367:GLY:HA3  | 6:Y:448:GLN:HB2  | 1.84                     | 0.60              |
| 6:Y:66:LYS:HB3   | 6:Y:69:GLU:HB2   | 1.83                     | 0.59              |
| 1:f:349:ILE:HD11 | 1:f:392:GLU:HG3  | 1.83                     | 0.59              |
| 5:X:1320:PRO:HG2 | 5:X:1323:PHE:HB2 | 1.85                     | 0.59              |
| 1:a:244:GLU:HA   | 1:a:247:ILE:HG22 | 1.84                     | 0.59              |
| 1:b:349:ILE:HD11 | 1:b:392:GLU:HG3  | 1.83                     | 0.59              |
| 6:Y:1263:LYS:HZ2 | 6:Y:1315:ALA:HB1 | 1.66                     | 0.59              |
| 5:X:314:ASN:ND2  | 5:X:348:SER:O    | 2.32                     | 0.59              |
| 6:Y:1075:ARG:HE  | 6:Y:1100:PHE:HB3 | 1.67                     | 0.59              |
| 1:d:24:GLU:CG    | 5:X:997:TRP:HH2  | 2.14                     | 0.59              |
| 1:f:244:GLU:HA   | 1:f:247:ILE:HG22 | 1.84                     | 0.59              |
| 4:W:26:ARG:HE    | 4:W:30:MET:HG2   | 1.67                     | 0.59              |
| 5:X:10:ARG:HH11  | 5:X:1181:PRO:CG  | 2.16                     | 0.59              |
| 5:X:808:ASN:H    | 6:Y:633:ALA:HB2  | 1.68                     | 0.59              |
| 1:e:349:ILE:HD11 | 1:e:392:GLU:HG3  | 1.83                     | 0.59              |
| 5:X:193:ASN:HD21 | 5:X:353:VAL:HG11 | 1.68                     | 0.59              |
| 5:X:682:GLY:HA2  | 5:X:685:MET:HE2  | 1.85                     | 0.59              |
| 6:Y:716:GLN:HG3  | 6:Y:718:SER:H    | 1.67                     | 0.59              |
| 1:b:49:ILE:HB    | 1:b:101:ILE:HG13 | 1.85                     | 0.59              |
| 1:e:207:LEU:HD23 | 1:e:264:LEU:HD12 | 1.83                     | 0.59              |
| 3:V:185:TYR:HB2  | 3:V:201:LEU:HD11 | 1.84                     | 0.59              |
| 6:Y:146:VAL:HG21 | 6:Y:154:LEU:HD13 | 1.83                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:Y:325:LYS:HG3   | 6:Y:329:ASP:HB2   | 1.85                     | 0.59              |
| 6:Y:836:ARG:NH1   | 6:Y:866:GLU:OE1   | 2.36                     | 0.59              |
| 6:Y:976:THR:HB    | 6:Y:1028:ILE:HD11 | 1.84                     | 0.59              |
| 7:K:9:DG:H2''     | 7:K:10:DA:C8      | 2.38                     | 0.59              |
| 1:a:49:ILE:HB     | 1:a:101:ILE:HG13  | 1.85                     | 0.59              |
| 1:d:49:ILE:HB     | 1:d:101:ILE:HG13  | 1.85                     | 0.59              |
| 5:X:143:ARG:HA    | 5:X:514:PHE:HA    | 1.85                     | 0.59              |
| 5:X:1185:PRO:HD2  | 5:X:1189:GLY:HA2  | 1.83                     | 0.59              |
| 6:Y:352:ARG:NH2   | 6:Y:465:GLN:OE1   | 2.35                     | 0.59              |
| 1:f:207:LEU:HD23  | 1:f:264:LEU:HD12  | 1.83                     | 0.58              |
| 3:U:321:TRP:CD1   | 3:U:322:PRO:HD3   | 2.38                     | 0.58              |
| 5:X:992:LEU:HG    | 5:X:993:PRO:HD3   | 1.84                     | 0.58              |
| 3:U:262:LEU:HD21  | 3:U:266:SER:HB3   | 1.84                     | 0.58              |
| 1:c:49:ILE:HB     | 1:c:101:ILE:HG13  | 1.85                     | 0.58              |
| 1:c:65:LEU:O      | 1:c:78:ASP:HA     | 2.03                     | 0.58              |
| 1:f:65:LEU:O      | 1:f:78:ASP:HA     | 2.03                     | 0.58              |
| 3:U:167:PRO:HG2   | 3:U:170:ARG:HD3   | 1.83                     | 0.58              |
| 6:Y:385:LEU:HD22  | 6:Y:390:LEU:HD23  | 1.85                     | 0.58              |
| 6:Y:746:LEU:HD23  | 6:Y:758:PRO:HB3   | 1.85                     | 0.58              |
| 1:d:65:LEU:O      | 1:d:78:ASP:HA     | 2.03                     | 0.58              |
| 1:d:140:HIS:O     | 1:d:306:ASN:ND2   | 2.26                     | 0.58              |
| 1:e:65:LEU:O      | 1:e:78:ASP:HA     | 2.03                     | 0.58              |
| 5:X:521:LEU:HD11  | 5:X:664:GLY:HA2   | 1.86                     | 0.58              |
| 6:Y:253:VAL:HB    | 6:Y:254:PRO:HD2   | 1.85                     | 0.58              |
| 6:Y:1347:LEU:HD22 | 6:Y:1357:ILE:HG23 | 1.86                     | 0.58              |
| 1:c:244:GLU:HA    | 1:c:247:ILE:HG22  | 1.84                     | 0.58              |
| 1:e:244:GLU:HA    | 1:e:247:ILE:HG22  | 1.84                     | 0.58              |
| 2:A:282:GLN:O     | 2:A:286:ASN:ND2   | 2.37                     | 0.58              |
| 6:Y:926:PRO:HB3   | 6:Y:1246:VAL:HG11 | 1.85                     | 0.58              |
| 1:d:90:ASN:HB3    | 1:e:28:ARG:HD3    | 1.86                     | 0.58              |
| 1:e:49:ILE:HB     | 1:e:101:ILE:HG13  | 1.85                     | 0.58              |
| 6:Y:701:LEU:HG    | 6:Y:723:TYR:HB2   | 1.84                     | 0.58              |
| 6:Y:1346:GLY:O    | 6:Y:1350:ASN:ND2  | 2.36                     | 0.58              |
| 5:X:1283:ALA:HB1  | 5:X:1286:THR:HB   | 1.86                     | 0.57              |
| 1:f:49:ILE:HB     | 1:f:101:ILE:HG13  | 1.85                     | 0.57              |
| 2:A:298:VAL:HG22  | 2:A:305:MET:HG2   | 1.85                     | 0.57              |
| 1:e:140:HIS:O     | 1:e:306:ASN:ND2   | 2.26                     | 0.57              |
| 6:Y:1190:ILE:HG23 | 6:Y:1194:ARG:HH21 | 1.69                     | 0.57              |
| 1:e:1:MET:N       | 1:e:5:GLU:OE2     | 2.31                     | 0.57              |
| 2:A:200:SER:HB3   | 2:A:230:PRO:HB3   | 1.85                     | 0.57              |
| 5:X:185:ASP:HB3   | 5:X:197:ARG:HG3   | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:X:1126:ASP:O    | 5:X:1127:LYS:C    | 2.47                     | 0.57              |
| 6:Y:816:THR:HG21  | 6:Y:889:ASP:HB2   | 1.87                     | 0.57              |
| 6:Y:850:LYS:NZ    | 6:Y:875:ASN:OD1   | 2.38                     | 0.57              |
| 6:Y:962:ASN:HB3   | 6:Y:964:LYS:NZ    | 2.18                     | 0.57              |
| 1:d:90:ASN:HB2    | 1:e:28:ARG:HD3    | 1.85                     | 0.57              |
| 2:A:260:GLN:O     | 2:A:264:THR:HG23  | 2.05                     | 0.57              |
| 1:a:65:LEU:O      | 1:a:78:ASP:HA     | 2.03                     | 0.57              |
| 3:V:13:LEU:HB3    | 3:V:28:LEU:HD23   | 1.87                     | 0.57              |
| 5:X:891:GLY:H     | 5:X:911:SER:HB3   | 1.68                     | 0.57              |
| 1:a:26:LEU:HB3    | 1:a:34:ILE:HG12   | 1.87                     | 0.57              |
| 1:d:26:LEU:HB3    | 1:d:34:ILE:HG12   | 1.87                     | 0.57              |
| 2:A:38:LYS:HD3    | 2:A:100:VAL:HB    | 1.86                     | 0.57              |
| 6:Y:495:ASN:ND2   | 6:Y:1247:LYS:O    | 2.33                     | 0.57              |
| 1:d:302:GLY:HA3   | 1:e:232:PHE:CZ    | 2.40                     | 0.57              |
| 1:e:26:LEU:HB3    | 1:e:34:ILE:HG12   | 1.87                     | 0.57              |
| 3:U:100:LEU:HD21  | 3:U:121:VAL:HG11  | 1.86                     | 0.57              |
| 4:W:60:ASN:H      | 4:W:63:ILE:HG22   | 1.69                     | 0.57              |
| 1:b:65:LEU:O      | 1:b:78:ASP:HA     | 2.03                     | 0.57              |
| 2:A:142:VAL:HG12  | 2:A:152:LEU:HG    | 1.86                     | 0.57              |
| 1:b:26:LEU:HB3    | 1:b:34:ILE:HG12   | 1.87                     | 0.56              |
| 2:A:24:PHE:O      | 2:A:28:GLU:HG2    | 2.04                     | 0.56              |
| 1:a:301:PHE:HE1   | 1:a:317:ALA:HB3   | 1.71                     | 0.56              |
| 1:e:378:GLN:O     | 1:e:382:ILE:HG23  | 2.06                     | 0.56              |
| 3:U:92:VAL:HG12   | 3:U:121:VAL:HG22  | 1.86                     | 0.56              |
| 5:X:816:ILE:HD13  | 5:X:1232:MET:HE1  | 1.87                     | 0.56              |
| 1:e:230:SER:HB2   | 1:e:242:VAL:HG21  | 1.88                     | 0.56              |
| 1:f:1:MET:N       | 1:f:5:GLU:OE2     | 2.31                     | 0.56              |
| 1:f:378:GLN:O     | 1:f:382:ILE:HG23  | 2.06                     | 0.56              |
| 5:X:1274:GLU:OE1  | 5:X:1274:GLU:N    | 2.39                     | 0.56              |
| 2:A:93:VAL:HG22   | 2:A:94:GLU:H      | 1.70                     | 0.56              |
| 6:Y:1156:LEU:HD12 | 6:Y:1223:LEU:HD11 | 1.87                     | 0.56              |
| 1:d:298:LYS:HE3   | 1:e:232:PHE:HB2   | 1.88                     | 0.56              |
| 1:f:301:PHE:HE1   | 1:f:317:ALA:HB3   | 1.71                     | 0.56              |
| 5:X:10:ARG:HH21   | 5:X:1175:ASN:HB3  | 1.71                     | 0.56              |
| 5:X:1066:MET:HG2  | 5:X:1076:ILE:HD11 | 1.88                     | 0.56              |
| 1:f:230:SER:HB2   | 1:f:242:VAL:HG21  | 1.88                     | 0.56              |
| 6:Y:279:LEU:HD23  | 6:Y:283:LEU:HD23  | 1.87                     | 0.56              |
| 1:a:230:SER:HB2   | 1:a:242:VAL:HG21  | 1.88                     | 0.56              |
| 1:b:301:PHE:HE1   | 1:b:317:ALA:HB3   | 1.71                     | 0.56              |
| 1:b:378:GLN:O     | 1:b:382:ILE:HG23  | 2.06                     | 0.56              |
| 1:c:378:GLN:O     | 1:c:382:ILE:HG23  | 2.06                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:26:LEU:HB3   | 1:f:34:ILE:HG12  | 1.87                     | 0.56              |
| 2:A:6:LEU:O      | 2:A:10:GLU:HG2   | 2.04                     | 0.56              |
| 3:U:101:THR:HG1  | 3:U:116:THR:HG1  | 1.54                     | 0.56              |
| 5:X:27:LEU:O     | 5:X:528:ARG:NH1  | 2.33                     | 0.56              |
| 1:d:230:SER:HB2  | 1:d:242:VAL:HG21 | 1.88                     | 0.55              |
| 1:f:102:ARG:NH1  | 2:A:131:ARG:HH22 | 2.04                     | 0.55              |
| 1:c:301:PHE:HE1  | 1:c:317:ALA:HB3  | 1.71                     | 0.55              |
| 5:X:421:SER:OG   | 5:X:423:ASP:OD1  | 2.25                     | 0.55              |
| 3:U:207:THR:HG23 | 3:U:209:GLY:H    | 1.71                     | 0.55              |
| 5:X:1004:ASP:HA  | 5:X:1008:GLN:HG2 | 1.88                     | 0.55              |
| 1:d:171:GLY:H    | 1:d:314:THR:HG1  | 1.53                     | 0.55              |
| 3:V:104:LYS:NZ   | 3:V:105:SER:O    | 2.34                     | 0.55              |
| 1:a:378:GLN:O    | 1:a:382:ILE:HG23 | 2.06                     | 0.55              |
| 5:X:122:VAL:HG23 | 5:X:490:GLN:HG2  | 1.88                     | 0.55              |
| 5:X:1247:SER:OG  | 6:Y:375:GLU:O    | 2.21                     | 0.55              |
| 1:b:92:ARG:NH1   | 1:b:255:GLU:OE2  | 2.40                     | 0.55              |
| 1:b:228:VAL:HG11 | 1:b:246:VAL:HG11 | 1.89                     | 0.55              |
| 1:c:92:ARG:NH1   | 1:c:255:GLU:OE2  | 2.40                     | 0.55              |
| 1:d:301:PHE:HE1  | 1:d:317:ALA:HB3  | 1.70                     | 0.55              |
| 1:e:301:PHE:HE1  | 1:e:317:ALA:HB3  | 1.71                     | 0.55              |
| 2:A:447:LYS:HE3  | 2:A:471:GLU:H    | 1.72                     | 0.55              |
| 6:Y:825:VAL:HG12 | 6:Y:833:GLU:HG2  | 1.89                     | 0.55              |
| 6:Y:1062:LEU:O   | 6:Y:1067:ARG:NH2 | 2.40                     | 0.55              |
| 1:a:92:ARG:NH1   | 1:a:255:GLU:OE2  | 2.40                     | 0.55              |
| 1:b:399:LEU:O    | 1:b:403:LEU:HB2  | 2.07                     | 0.55              |
| 2:A:224:LYS:HG2  | 2:A:276:TRP:CD2  | 2.42                     | 0.55              |
| 1:f:92:ARG:NH1   | 1:f:255:GLU:OE2  | 2.40                     | 0.55              |
| 4:W:25:ARG:HD2   | 4:W:64:LEU:HD21  | 1.88                     | 0.55              |
| 1:c:1:MET:N      | 1:c:5:GLU:OE2    | 2.31                     | 0.55              |
| 1:c:26:LEU:HB3   | 1:c:34:ILE:HG12  | 1.87                     | 0.55              |
| 1:c:230:SER:HB2  | 1:c:242:VAL:HG21 | 1.88                     | 0.55              |
| 1:d:399:LEU:O    | 1:d:403:LEU:HB2  | 2.07                     | 0.55              |
| 1:e:92:ARG:NH1   | 1:e:255:GLU:OE2  | 2.40                     | 0.55              |
| 1:e:228:VAL:HG11 | 1:e:246:VAL:HG11 | 1.89                     | 0.55              |
| 1:f:399:LEU:O    | 1:f:403:LEU:HB2  | 2.07                     | 0.55              |
| 2:A:203:GLU:HA   | 2:A:206:ILE:HG12 | 1.89                     | 0.55              |
| 6:Y:747:MET:HE2  | 6:Y:775:SER:HA   | 1.88                     | 0.55              |
| 6:Y:842:ARG:NH2  | 6:Y:883:ARG:O    | 2.37                     | 0.55              |
| 6:Y:1256:ILE:O   | 6:Y:1260:MET:HG2 | 2.07                     | 0.55              |
| 1:a:138:PRO:HB3  | 1:a:305:ARG:HB2  | 1.90                     | 0.54              |
| 1:a:399:LEU:O    | 1:a:403:LEU:HB2  | 2.07                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:b:179:PRO:HB2   | 1:b:347:ARG:HD2   | 1.90                     | 0.54              |
| 1:b:230:SER:HB2   | 1:b:242:VAL:HG21  | 1.88                     | 0.54              |
| 1:d:92:ARG:NH1    | 1:d:255:GLU:OE2   | 2.40                     | 0.54              |
| 1:d:235:PRO:HD2   | 1:d:238:ARG:HD3   | 1.89                     | 0.54              |
| 2:A:2:ASN:HB2     | 2:A:55:ASP:HB3    | 1.90                     | 0.54              |
| 6:Y:144:TYR:OH    | 6:Y:293:ARG:NH1   | 2.34                     | 0.54              |
| 6:Y:1358:PRO:HA   | 6:Y:1363:TYR:HA   | 1.89                     | 0.54              |
| 1:a:160:ARG:NH2   | 1:a:408:THR:O     | 2.41                     | 0.54              |
| 1:a:179:PRO:HB2   | 1:a:347:ARG:HD2   | 1.89                     | 0.54              |
| 1:b:160:ARG:NH2   | 1:b:408:THR:O     | 2.41                     | 0.54              |
| 1:c:399:LEU:O     | 1:c:403:LEU:HB2   | 2.07                     | 0.54              |
| 1:d:378:GLN:O     | 1:d:382:ILE:HG23  | 2.06                     | 0.54              |
| 5:X:557:ARG:NH2   | 5:X:611:GLU:OE2   | 2.40                     | 0.54              |
| 5:X:993:PRO:HB2   | 5:X:997:TRP:CD1   | 2.42                     | 0.54              |
| 6:Y:750:PRO:HG3   | 6:Y:777:HIS:HE1   | 1.72                     | 0.54              |
| 1:a:235:PRO:HD2   | 1:a:238:ARG:HD3   | 1.90                     | 0.54              |
| 3:V:181:GLU:HB3   | 3:V:206:GLU:OE1   | 2.07                     | 0.54              |
| 1:c:171:GLY:H     | 1:c:314:THR:HG1   | 1.55                     | 0.54              |
| 2:A:22:LYS:HB3    | 2:A:117:LYS:NZ    | 2.23                     | 0.54              |
| 2:A:168:LEU:HB2   | 2:A:171:GLU:HB2   | 1.90                     | 0.54              |
| 5:X:594:VAL:HG22  | 5:X:599:VAL:HG13  | 1.89                     | 0.54              |
| 5:X:709:ALA:HB2   | 5:X:794:LEU:HB2   | 1.88                     | 0.54              |
| 5:X:1323:PHE:O    | 5:X:1326:LEU:HG   | 2.08                     | 0.54              |
| 6:Y:1046:ILE:HG22 | 6:Y:1061:VAL:HG22 | 1.89                     | 0.54              |
| 1:c:179:PRO:HB2   | 1:c:347:ARG:HD2   | 1.90                     | 0.54              |
| 1:c:185:THR:HA    | 1:c:188:LEU:HD12  | 1.90                     | 0.54              |
| 11:d:1000:ADP:O2B | 10:d:1002:BEF:F3  | 2.16                     | 0.54              |
| 1:f:138:PRO:HB3   | 1:f:305:ARG:HB2   | 1.90                     | 0.54              |
| 3:U:237:VAL:HG22  | 3:V:13:LEU:HG     | 1.89                     | 0.54              |
| 6:Y:370:LYS:HG2   | 6:Y:441:LEU:HD12  | 1.90                     | 0.54              |
| 6:Y:848:VAL:HB    | 6:Y:858:VAL:HB    | 1.90                     | 0.54              |
| 1:e:235:PRO:HD2   | 1:e:238:ARG:HD3   | 1.90                     | 0.54              |
| 5:X:246:LEU:HD12  | 5:X:249:GLU:HB2   | 1.88                     | 0.54              |
| 1:a:228:VAL:HG11  | 1:a:246:VAL:HG11  | 1.89                     | 0.54              |
| 1:f:228:VAL:HG11  | 1:f:246:VAL:HG11  | 1.89                     | 0.54              |
| 1:c:235:PRO:HD2   | 1:c:238:ARG:HD3   | 1.89                     | 0.54              |
| 1:d:135:ASN:CB    | 1:e:11:VAL:HG11   | 2.36                     | 0.54              |
| 1:d:178:ALA:HB3   | 1:d:184:LYS:HE3   | 1.90                     | 0.54              |
| 1:f:235:PRO:HD2   | 1:f:238:ARG:HD3   | 1.89                     | 0.54              |
| 5:X:263:VAL:HG21  | 5:X:269:ILE:HD11  | 1.88                     | 0.54              |
| 5:X:896:THR:HG22  | 5:X:898:GLU:H     | 1.72                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:X:1122:LYS:HG2  | 5:X:1229:TYR:CZ   | 2.43                     | 0.54              |
| 1:b:185:THR:HA    | 1:b:188:LEU:HD12  | 1.90                     | 0.54              |
| 1:c:106:GLU:OE1   | 1:c:106:GLU:N     | 2.35                     | 0.54              |
| 1:f:294:LEU:C     | 1:f:297:PRO:HD2   | 2.33                     | 0.54              |
| 4:W:20:VAL:HG11   | 6:Y:1361:THR:HG21 | 1.89                     | 0.54              |
| 1:e:138:PRO:HB3   | 1:e:305:ARG:HB2   | 1.90                     | 0.53              |
| 1:e:160:ARG:NH2   | 1:e:408:THR:O     | 2.41                     | 0.53              |
| 1:f:160:ARG:NH2   | 1:f:408:THR:O     | 2.41                     | 0.53              |
| 1:f:184:LYS:H     | 11:f:1000:ADP:PB  | 2.31                     | 0.53              |
| 2:A:123:ARG:NH1   | 2:A:192:GLY:O     | 2.41                     | 0.53              |
| 3:U:184:ALA:HB2   | 5:X:1091:GLY:HA3  | 1.90                     | 0.53              |
| 4:W:31:GLN:NE2    | 5:X:1311:GLY:O    | 2.39                     | 0.53              |
| 1:a:185:THR:HA    | 1:a:188:LEU:HD12  | 1.90                     | 0.53              |
| 1:c:59:GLN:OE1    | 1:c:59:GLN:N      | 2.27                     | 0.53              |
| 1:c:160:ARG:NH2   | 1:c:408:THR:O     | 2.41                     | 0.53              |
| 1:c:228:VAL:HG11  | 1:c:246:VAL:HG11  | 1.89                     | 0.53              |
| 1:e:399:LEU:O     | 1:e:403:LEU:HB2   | 2.07                     | 0.53              |
| 11:e:1000:ADP:O2B | 10:e:1002:BEF:F3  | 2.16                     | 0.53              |
| 6:Y:393:THR:HG23  | 6:Y:396:ALA:H     | 1.72                     | 0.53              |
| 6:Y:514:THR:HG21  | 6:Y:596:LEU:HD23  | 1.89                     | 0.53              |
| 1:d:228:VAL:HG11  | 1:d:246:VAL:HG11  | 1.89                     | 0.53              |
| 5:X:255:ILE:HB    | 5:X:263:VAL:HB    | 1.90                     | 0.53              |
| 5:X:812:PHE:HB3   | 6:Y:357:VAL:HG11  | 1.90                     | 0.53              |
| 6:Y:830:ASP:OD1   | 6:Y:831:VAL:N     | 2.32                     | 0.53              |
| 1:b:138:PRO:HB3   | 1:b:305:ARG:HB2   | 1.90                     | 0.53              |
| 1:b:409:ASN:OD1   | 1:b:409:ASN:N     | 2.41                     | 0.53              |
| 1:d:59:GLN:OE1    | 1:d:59:GLN:N      | 2.27                     | 0.53              |
| 1:d:185:THR:HA    | 1:d:188:LEU:HD12  | 1.90                     | 0.53              |
| 1:e:294:LEU:C     | 1:e:297:PRO:HD2   | 2.33                     | 0.53              |
| 1:f:179:PRO:HB2   | 1:f:347:ARG:HD2   | 1.90                     | 0.53              |
| 5:X:517:GLN:HA    | 5:X:523:GLU:OE2   | 2.08                     | 0.53              |
| 6:Y:337:ARG:NH1   | 6:Y:341:ASN:OD1   | 2.41                     | 0.53              |
| 1:b:59:GLN:OE1    | 1:b:59:GLN:N      | 2.27                     | 0.53              |
| 1:b:178:ALA:HB3   | 1:b:184:LYS:HE3   | 1.90                     | 0.53              |
| 1:d:294:LEU:C     | 1:d:297:PRO:HD2   | 2.33                     | 0.53              |
| 6:Y:1002:VAL:HB   | 6:Y:1019:ASN:HB2  | 1.91                     | 0.53              |
| 1:c:409:ASN:OD1   | 1:c:409:ASN:N     | 2.41                     | 0.53              |
| 1:d:1:MET:N       | 1:d:5:GLU:OE2     | 2.31                     | 0.53              |
| 1:d:179:PRO:HB2   | 1:d:347:ARG:HD2   | 1.90                     | 0.53              |
| 1:f:158:THR:HA    | 1:f:356:PRO:HG3   | 1.91                     | 0.53              |
| 1:a:178:ALA:HB3   | 1:a:184:LYS:HE3   | 1.90                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:e:114:LEU:HD12 | 2:A:84:ASP:HB2    | 1.90                     | 0.53              |
| 6:Y:643:ASP:O    | 6:Y:720:ASN:ND2   | 2.42                     | 0.53              |
| 1:a:294:LEU:C    | 1:a:297:PRO:HD2   | 2.33                     | 0.53              |
| 1:b:158:THR:HA   | 1:b:356:PRO:HG3   | 1.91                     | 0.53              |
| 1:e:179:PRO:HB2  | 1:e:347:ARG:HD2   | 1.90                     | 0.53              |
| 2:A:149:ASN:HB3  | 2:A:163:LEU:HD13  | 1.91                     | 0.53              |
| 3:V:71:LYS:NZ    | 3:V:72:GLU:O      | 2.40                     | 0.53              |
| 5:X:1157:GLN:HG3 | 5:X:1159:VAL:HG13 | 1.90                     | 0.53              |
| 6:Y:180:MET:HE1  | 6:Y:293:ARG:HG2   | 1.91                     | 0.53              |
| 9:R:91:G:H2'     | 9:R:92:C:C6       | 2.43                     | 0.53              |
| 1:b:235:PRO:HD2  | 1:b:238:ARG:HD3   | 1.90                     | 0.53              |
| 1:d:160:ARG:NH2  | 1:d:408:THR:O     | 2.41                     | 0.53              |
| 1:e:7:LYS:NZ     | 1:e:77:ASP:OD2    | 2.42                     | 0.53              |
| 1:f:185:THR:HA   | 1:f:188:LEU:HD12  | 1.90                     | 0.53              |
| 1:c:138:PRO:HB3  | 1:c:305:ARG:HB2   | 1.90                     | 0.53              |
| 2:A:400:GLU:O    | 2:A:404:GLU:HG3   | 2.09                     | 0.53              |
| 5:X:964:LEU:HD21 | 5:X:1022:LYS:HE3  | 1.91                     | 0.53              |
| 6:Y:1172:LYS:HD2 | 6:Y:1191:PRO:HA   | 1.91                     | 0.53              |
| 1:b:1:MET:N      | 1:b:5:GLU:OE2     | 2.31                     | 0.52              |
| 1:c:294:LEU:C    | 1:c:297:PRO:HD2   | 2.33                     | 0.52              |
| 1:f:7:LYS:NZ     | 1:f:77:ASP:OD2    | 2.42                     | 0.52              |
| 1:d:138:PRO:HB3  | 1:d:305:ARG:HB2   | 1.90                     | 0.52              |
| 1:d:341:MET:HE3  | 1:d:343:LEU:HD11  | 1.92                     | 0.52              |
| 5:X:806:PRO:HA   | 5:X:811:ASN:HD21  | 1.73                     | 0.52              |
| 6:Y:686:TRP:CD2  | 6:Y:758:PRO:HG3   | 2.44                     | 0.52              |
| 3:U:113:ALA:HB2  | 3:U:126:PRO:HB2   | 1.90                     | 0.52              |
| 3:V:61:ILE:HG22  | 3:V:63:GLY:H      | 1.74                     | 0.52              |
| 1:b:341:MET:HE3  | 1:b:343:LEU:HD11  | 1.92                     | 0.52              |
| 1:c:406:THR:HG21 | 1:c:412:PHE:HB2   | 1.92                     | 0.52              |
| 1:e:185:THR:HA   | 1:e:188:LEU:HD12  | 1.90                     | 0.52              |
| 3:V:193:GLU:HG2  | 3:V:194:GLN:N     | 2.23                     | 0.52              |
| 6:Y:438:GLU:HG3  | 6:Y:485:MET:HE1   | 1.91                     | 0.52              |
| 1:e:158:THR:HA   | 1:e:356:PRO:HG3   | 1.91                     | 0.52              |
| 5:X:935:THR:HG21 | 5:X:941:LYS:HG2   | 1.90                     | 0.52              |
| 6:Y:107:LEU:HD21 | 6:Y:299:LEU:HD21  | 1.91                     | 0.52              |
| 1:a:158:THR:HA   | 1:a:356:PRO:HG3   | 1.91                     | 0.52              |
| 1:b:31:LYS:HA    | 1:b:34:ILE:HD12   | 1.92                     | 0.52              |
| 1:e:341:MET:HE3  | 1:e:343:LEU:HD11  | 1.92                     | 0.52              |
| 5:X:820:GLU:N    | 5:X:1080:ASN:O    | 2.40                     | 0.52              |
| 5:X:1269:ARG:HA  | 6:Y:346:ARG:HA    | 1.91                     | 0.52              |
| 6:Y:491:LEU:HB3  | 6:Y:904:ALA:HA    | 1.90                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:b:7:LYS:NZ     | 1:b:77:ASP:OD2    | 2.42                     | 0.52              |
| 1:f:178:ALA:HB3  | 1:f:184:LYS:HE3   | 1.90                     | 0.52              |
| 3:V:37:HIS:CE1   | 5:X:1216:ARG:HD2  | 2.45                     | 0.52              |
| 5:X:674:ASP:OD2  | 5:X:1070:HIS:ND1  | 2.38                     | 0.52              |
| 6:Y:363:LEU:HD23 | 6:Y:618:VAL:HG13  | 1.90                     | 0.52              |
| 1:a:409:ASN:OD1  | 1:a:409:ASN:N     | 2.41                     | 0.52              |
| 2:A:327:LEU:O    | 2:A:331:LEU:N     | 2.43                     | 0.52              |
| 1:b:294:LEU:C    | 1:b:297:PRO:HD2   | 2.33                     | 0.52              |
| 1:c:31:LYS:HA    | 1:c:34:ILE:HD12   | 1.92                     | 0.52              |
| 1:c:158:THR:HA   | 1:c:356:PRO:HG3   | 1.91                     | 0.52              |
| 1:d:158:THR:HA   | 1:d:356:PRO:HG3   | 1.91                     | 0.52              |
| 5:X:227:LYS:HD2  | 5:X:334:GLU:HB3   | 1.92                     | 0.52              |
| 1:a:7:LYS:NZ     | 1:a:77:ASP:OD2    | 2.42                     | 0.52              |
| 1:a:394:ASP:HA   | 1:a:397:GLU:HB2   | 1.92                     | 0.52              |
| 1:e:178:ALA:HB3  | 1:e:184:LYS:HE3   | 1.90                     | 0.52              |
| 1:e:406:THR:HG21 | 1:e:412:PHE:HB2   | 1.92                     | 0.52              |
| 1:f:394:ASP:HA   | 1:f:397:GLU:HB2   | 1.92                     | 0.52              |
| 5:X:1289:GLU:HG2 | 5:X:1315:MET:HG3  | 1.92                     | 0.52              |
| 8:L:-6:DC:H2'    | 8:L:-5:DT:H71     | 1.92                     | 0.52              |
| 1:a:31:LYS:HA    | 1:a:34:ILE:HD12   | 1.92                     | 0.51              |
| 1:c:7:LYS:NZ     | 1:c:77:ASP:OD2    | 2.42                     | 0.51              |
| 1:f:406:THR:HG21 | 1:f:412:PHE:HB2   | 1.92                     | 0.51              |
| 3:U:16:ILE:HG12  | 3:U:214:GLU:HB2   | 1.92                     | 0.51              |
| 5:X:11:ILE:HG12  | 5:X:1159:VAL:HG11 | 1.92                     | 0.51              |
| 5:X:69:GLN:HB2   | 5:X:101:ARG:HB3   | 1.92                     | 0.51              |
| 5:X:582:ASN:HB3  | 5:X:586:PHE:H     | 1.75                     | 0.51              |
| 1:d:406:THR:HG21 | 1:d:412:PHE:HB2   | 1.92                     | 0.51              |
| 3:V:99:ILE:HG22  | 3:V:145:LYS:HG3   | 1.91                     | 0.51              |
| 3:V:182:ARG:HB3  | 6:Y:531:LYS:HB3   | 1.92                     | 0.51              |
| 5:X:144:VAL:HG21 | 5:X:527:LYS:HG2   | 1.92                     | 0.51              |
| 5:X:826:ASP:OD1  | 5:X:829:THR:OG1   | 2.24                     | 0.51              |
| 9:R:94:U:H2'     | 9:R:95:G:H8       | 1.74                     | 0.51              |
| 1:f:171:GLY:H    | 1:f:314:THR:HG1   | 1.54                     | 0.51              |
| 6:Y:210:SER:HB3  | 6:Y:213:LYS:HG2   | 1.92                     | 0.51              |
| 6:Y:332:LYS:HD3  | 6:Y:1329:THR:HG23 | 1.92                     | 0.51              |
| 6:Y:865:HIS:H    | 6:Y:868:TRP:CD1   | 2.28                     | 0.51              |
| 8:L:4:DC:H2'     | 8:L:5:DA:H8       | 1.74                     | 0.51              |
| 1:a:1:MET:N      | 1:a:5:GLU:OE2     | 2.31                     | 0.51              |
| 1:b:394:ASP:HA   | 1:b:397:GLU:HB2   | 1.92                     | 0.51              |
| 3:U:182:ARG:HG2  | 3:U:206:GLU:HB3   | 1.93                     | 0.51              |
| 5:X:10:ARG:NH1   | 5:X:697:LYS:HD3   | 2.25                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:a:341:MET:HE3  | 1:a:343:LEU:HD11  | 1.92                     | 0.51              |
| 1:b:65:LEU:HB2   | 1:b:79:ILE:HB     | 1.92                     | 0.51              |
| 1:c:173:ARG:O    | 1:c:341:MET:HB3   | 2.11                     | 0.51              |
| 1:c:178:ALA:HB3  | 1:c:184:LYS:HE3   | 1.90                     | 0.51              |
| 1:d:7:LYS:NZ     | 1:d:77:ASP:OD2    | 2.42                     | 0.51              |
| 1:d:31:LYS:HA    | 1:d:34:ILE:HD12   | 1.92                     | 0.51              |
| 5:X:1281:TYR:HD2 | 6:Y:484:MET:HE3   | 1.75                     | 0.51              |
| 1:c:341:MET:HE3  | 1:c:343:LEU:HD11  | 1.92                     | 0.51              |
| 1:d:156:ASP:O    | 1:d:157:LEU:C     | 2.54                     | 0.51              |
| 1:f:102:ARG:HH22 | 2:A:131:ARG:HH12  | 1.59                     | 0.51              |
| 1:f:173:ARG:O    | 1:f:341:MET:HB3   | 2.11                     | 0.51              |
| 3:V:91:ARG:NH1   | 3:V:210:THR:O     | 2.43                     | 0.51              |
| 6:Y:40:LYS:NZ    | 6:Y:54:ASP:OD1    | 2.33                     | 0.51              |
| 1:e:31:LYS:HA    | 1:e:34:ILE:HD12   | 1.92                     | 0.51              |
| 2:A:48:GLN:NE2   | 2:A:57:ASP:O      | 2.44                     | 0.51              |
| 3:U:225:ALA:HB2  | 3:V:232:VAL:HG11  | 1.92                     | 0.51              |
| 3:U:263:THR:HG22 | 3:U:264:VAL:H     | 1.75                     | 0.51              |
| 3:V:237:VAL:HG23 | 3:V:239:GLN:H     | 1.74                     | 0.51              |
| 7:K:11:DT:H2''   | 7:K:12:DA:C8      | 2.46                     | 0.51              |
| 1:e:394:ASP:HA   | 1:e:397:GLU:HB2   | 1.92                     | 0.51              |
| 3:U:27:THR:HG22  | 3:U:202:VAL:HG22  | 1.93                     | 0.51              |
| 5:X:72:SER:OG    | 5:X:73:TYR:N      | 2.43                     | 0.51              |
| 5:X:118:LYS:NZ   | 5:X:487:LEU:O     | 2.34                     | 0.51              |
| 5:X:883:LEU:HD11 | 5:X:1052:VAL:HG21 | 1.93                     | 0.51              |
| 9:R:94:U:H2'     | 9:R:95:G:C8       | 2.45                     | 0.51              |
| 1:a:62:PHE:CE2   | 8:L:20:DC:H4'     | 2.45                     | 0.51              |
| 1:c:3:LEU:HD12   | 1:c:7:LYS:HE2     | 1.93                     | 0.51              |
| 1:e:65:LEU:HB2   | 1:e:79:ILE:HB     | 1.92                     | 0.51              |
| 3:V:193:GLU:HG2  | 3:V:194:GLN:H     | 1.76                     | 0.51              |
| 6:Y:1167:LYS:HD2 | 6:Y:1170:LYS:HD2  | 1.92                     | 0.51              |
| 1:b:173:ARG:O    | 1:b:341:MET:HB3   | 2.11                     | 0.51              |
| 1:e:173:ARG:O    | 1:e:341:MET:HB3   | 2.11                     | 0.51              |
| 3:U:95:LYS:NZ    | 3:U:120:ASP:OD2   | 2.37                     | 0.51              |
| 5:X:1168:GLU:HA  | 5:X:1171:ARG:HD3  | 1.93                     | 0.51              |
| 6:Y:968:ASN:HA   | 6:Y:1117:SER:HB2  | 1.91                     | 0.51              |
| 1:b:406:THR:HG21 | 1:b:412:PHE:HB2   | 1.92                     | 0.50              |
| 1:d:106:GLU:OE1  | 1:d:106:GLU:N     | 2.35                     | 0.50              |
| 1:d:394:ASP:HA   | 1:d:397:GLU:HB2   | 1.92                     | 0.50              |
| 1:e:302:GLY:HA3  | 1:f:232:PHE:CE1   | 2.46                     | 0.50              |
| 1:f:31:LYS:HA    | 1:f:34:ILE:HD12   | 1.92                     | 0.50              |
| 3:U:227:GLN:HE21 | 3:V:35:PHE:HD2    | 1.59                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:a:173:ARG:O    | 1:a:341:MET:HB3   | 2.11                     | 0.50              |
| 1:a:406:THR:HG21 | 1:a:412:PHE:HB2   | 1.92                     | 0.50              |
| 1:d:65:LEU:HB2   | 1:d:79:ILE:HB     | 1.92                     | 0.50              |
| 1:e:106:GLU:OE1  | 1:e:106:GLU:N     | 2.35                     | 0.50              |
| 1:e:187:LEU:O    | 1:e:191:ILE:HG12  | 2.11                     | 0.50              |
| 1:e:273:ALA:O    | 1:e:277:VAL:HG13  | 2.12                     | 0.50              |
| 2:A:71:PRO:HG2   | 3:U:304:LYS:HB3   | 1.93                     | 0.50              |
| 3:U:228:LEU:HD11 | 3:V:224:LEU:HD23  | 1.92                     | 0.50              |
| 5:X:11:ILE:O     | 5:X:1149:TYR:OH   | 2.19                     | 0.50              |
| 5:X:160:ASP:HB3  | 5:X:164:THR:HG21  | 1.93                     | 0.50              |
| 5:X:764:CYS:HB2  | 5:X:833:ILE:HG13  | 1.92                     | 0.50              |
| 6:Y:965:SER:OG   | 6:Y:974:VAL:O     | 2.26                     | 0.50              |
| 6:Y:1132:LYS:HE2 | 6:Y:1152:GLU:HB3  | 1.91                     | 0.50              |
| 1:b:207:LEU:HD22 | 1:b:246:VAL:HG21  | 1.94                     | 0.50              |
| 1:c:65:LEU:HB2   | 1:c:79:ILE:HB     | 1.92                     | 0.50              |
| 1:c:187:LEU:O    | 1:c:191:ILE:HG12  | 2.11                     | 0.50              |
| 1:f:207:LEU:HD22 | 1:f:246:VAL:HG21  | 1.94                     | 0.50              |
| 2:A:166:ASP:HB3  | 2:A:198:THR:HA    | 1.93                     | 0.50              |
| 5:X:210:LEU:HD22 | 5:X:220:ILE:HG12  | 1.93                     | 0.50              |
| 5:X:453:ILE:HD11 | 5:X:581:THR:HG23  | 1.93                     | 0.50              |
| 6:Y:1136:GLY:HA2 | 6:Y:1140:ARG:HB2  | 1.94                     | 0.50              |
| 1:a:207:LEU:HD22 | 1:a:246:VAL:HG21  | 1.94                     | 0.50              |
| 1:b:156:ASP:O    | 1:b:157:LEU:C     | 2.54                     | 0.50              |
| 1:b:372:THR:HG23 | 1:b:376:GLU:HB3   | 1.94                     | 0.50              |
| 1:f:106:GLU:OE1  | 1:f:106:GLU:N     | 2.35                     | 0.50              |
| 1:f:341:MET:HE3  | 1:f:343:LEU:HD11  | 1.92                     | 0.50              |
| 3:U:238:ARG:NE   | 3:V:14:VAL:O      | 2.44                     | 0.50              |
| 3:V:215:GLU:OE2  | 3:V:219:ARG:NH2   | 2.43                     | 0.50              |
| 5:X:230:PHE:HB2  | 5:X:333:ILE:HB    | 1.92                     | 0.50              |
| 5:X:925:SER:OG   | 5:X:926:GLY:N     | 2.44                     | 0.50              |
| 5:X:1234:LYS:HE3 | 5:X:1238:LEU:HD21 | 1.93                     | 0.50              |
| 1:c:372:THR:HG23 | 1:c:376:GLU:HB3   | 1.94                     | 0.50              |
| 1:d:173:ARG:O    | 1:d:341:MET:HB3   | 2.11                     | 0.50              |
| 1:d:187:LEU:O    | 1:d:191:ILE:HG12  | 2.11                     | 0.50              |
| 1:e:73:LEU:HD22  | 1:e:238:ARG:HH21  | 1.77                     | 0.50              |
| 1:f:273:ALA:O    | 1:f:277:VAL:HG13  | 2.12                     | 0.50              |
| 3:U:316:MET:HG3  | 3:U:317:ARG:H     | 1.75                     | 0.50              |
| 4:W:15:ASN:HD21  | 4:W:18:ASP:HB2    | 1.75                     | 0.50              |
| 6:Y:503:SER:OG   | 6:Y:504:GLN:N     | 2.44                     | 0.50              |
| 1:a:3:LEU:HD12   | 1:a:7:LYS:HE2     | 1.93                     | 0.50              |
| 1:a:401:ASN:O    | 1:a:405:MET:HG2   | 2.12                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:b:273:ALA:O     | 1:b:277:VAL:HG13  | 2.12                     | 0.50              |
| 1:e:372:THR:HG23  | 1:e:376:GLU:HB3   | 1.94                     | 0.50              |
| 6:Y:818:GLU:HG2   | 6:Y:887:SER:HB2   | 1.92                     | 0.50              |
| 9:R:91:G:H2'      | 9:R:92:C:H6       | 1.76                     | 0.50              |
| 1:a:187:LEU:O     | 1:a:191:ILE:HG12  | 2.11                     | 0.50              |
| 1:b:401:ASN:O     | 1:b:405:MET:HG2   | 2.12                     | 0.50              |
| 1:c:128:ARG:HA    | 1:d:28:ARG:HD2    | 1.94                     | 0.50              |
| 1:c:156:ASP:O     | 1:c:157:LEU:C     | 2.54                     | 0.50              |
| 1:e:59:GLN:OE1    | 1:e:59:GLN:N      | 2.27                     | 0.50              |
| 1:f:187:LEU:O     | 1:f:191:ILE:HG12  | 2.11                     | 0.50              |
| 5:X:957:LYS:HE2   | 5:X:1029:LEU:HD11 | 1.94                     | 0.50              |
| 5:X:1260:GLY:O    | 5:X:1264:GLN:NE2  | 2.44                     | 0.50              |
| 8:L:1:DT:H2'      | 8:L:2:DG:H8       | 1.75                     | 0.50              |
| 1:a:273:ALA:O     | 1:a:277:VAL:HG13  | 2.12                     | 0.50              |
| 1:c:394:ASP:HA    | 1:c:397:GLU:HB2   | 1.92                     | 0.50              |
| 1:d:10:PRO:HG2    | 1:d:13:GLU:HB2    | 1.94                     | 0.50              |
| 1:d:73:LEU:HD22   | 1:d:238:ARG:HH21  | 1.77                     | 0.50              |
| 1:d:135:ASN:HB3   | 1:e:11:VAL:CG1    | 2.39                     | 0.50              |
| 1:d:207:LEU:HD22  | 1:d:246:VAL:HG21  | 1.94                     | 0.50              |
| 2:A:31:LEU:HD13   | 2:A:47:VAL:HG21   | 1.93                     | 0.50              |
| 6:Y:848:VAL:HG12  | 6:Y:857:LEU:HD21  | 1.94                     | 0.50              |
| 7:K:5:DA:H2''     | 7:K:6:DG:C8       | 2.47                     | 0.50              |
| 1:a:65:LEU:HB2    | 1:a:79:ILE:HB     | 1.92                     | 0.50              |
| 1:a:73:LEU:HD22   | 1:a:238:ARG:HH21  | 1.77                     | 0.50              |
| 1:a:372:THR:HG23  | 1:a:376:GLU:HB3   | 1.94                     | 0.50              |
| 1:c:73:LEU:HD22   | 1:c:238:ARG:HH21  | 1.77                     | 0.50              |
| 1:c:207:LEU:HD22  | 1:c:246:VAL:HG21  | 1.94                     | 0.50              |
| 1:c:273:ALA:O     | 1:c:277:VAL:HG13  | 2.12                     | 0.50              |
| 3:U:69:SER:OG     | 3:U:70:THR:N      | 2.44                     | 0.50              |
| 5:X:1113:LEU:HD21 | 6:Y:641:ILE:HD13  | 1.94                     | 0.50              |
| 6:Y:1027:VAL:O    | 6:Y:1120:THR:HA   | 2.12                     | 0.50              |
| 1:a:156:ASP:O     | 1:a:157:LEU:C     | 2.54                     | 0.49              |
| 1:a:205:MET:HE1   | 1:a:249:LYS:HD3   | 1.94                     | 0.49              |
| 1:b:10:PRO:HG2    | 1:b:13:GLU:HB2    | 1.94                     | 0.49              |
| 1:b:187:LEU:O     | 1:b:191:ILE:HG12  | 2.11                     | 0.49              |
| 1:d:372:THR:HG23  | 1:d:376:GLU:HB3   | 1.94                     | 0.49              |
| 1:f:205:MET:HE1   | 1:f:249:LYS:HD3   | 1.94                     | 0.49              |
| 5:X:196:VAL:HG11  | 5:X:209:ILE:HG21  | 1.93                     | 0.49              |
| 5:X:239:MET:HG2   | 5:X:240:GLU:O     | 2.11                     | 0.49              |
| 6:Y:1140:ARG:HG2  | 6:Y:1240:VAL:HG21 | 1.94                     | 0.49              |
| 1:d:273:ALA:O     | 1:d:277:VAL:HG13  | 2.12                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:e:156:ASP:O     | 1:e:157:LEU:C    | 2.54                     | 0.49              |
| 1:a:10:PRO:HG2    | 1:a:13:GLU:HB2   | 1.94                     | 0.49              |
| 1:e:3:LEU:HD12    | 1:e:7:LYS:HE2    | 1.93                     | 0.49              |
| 1:e:207:LEU:HD22  | 1:e:246:VAL:HG21 | 1.94                     | 0.49              |
| 1:f:65:LEU:HB2    | 1:f:79:ILE:HB    | 1.92                     | 0.49              |
| 1:f:372:THR:HG23  | 1:f:376:GLU:HB3  | 1.94                     | 0.49              |
| 5:X:1244:HIS:NE2  | 5:X:1266:GLY:O   | 2.42                     | 0.49              |
| 5:X:1269:ARG:HH22 | 6:Y:340:GLN:HA   | 1.77                     | 0.49              |
| 5:X:1288:GLN:NE2  | 5:X:1315:MET:HE1 | 2.27                     | 0.49              |
| 1:b:388:HIS:CE1   | 1:c:351:GLU:OE1  | 2.64                     | 0.49              |
| 1:d:3:LEU:HD12    | 1:d:7:LYS:HE2    | 1.93                     | 0.49              |
| 1:f:3:LEU:HD12    | 1:f:7:LYS:HE2    | 1.93                     | 0.49              |
| 3:V:91:ARG:HG3    | 3:V:122:GLU:HB3  | 1.94                     | 0.49              |
| 6:Y:119:SER:OG    | 6:Y:121:PRO:O    | 2.24                     | 0.49              |
| 6:Y:527:LEU:HD21  | 6:Y:533:ALA:HB2  | 1.93                     | 0.49              |
| 1:d:205:MET:HE1   | 1:d:249:LYS:HD3  | 1.94                     | 0.49              |
| 1:d:409:ASN:OD1   | 1:d:409:ASN:N    | 2.41                     | 0.49              |
| 1:f:401:ASN:O     | 1:f:405:MET:HG2  | 2.12                     | 0.49              |
| 3:V:134:THR:HG22  | 3:V:136:GLU:H    | 1.78                     | 0.49              |
| 3:V:192:VAL:HG22  | 3:V:193:GLU:H    | 1.77                     | 0.49              |
| 5:X:742:TYR:HB2   | 5:X:746:ALA:HB2  | 1.93                     | 0.49              |
| 6:Y:58:CYS:SG     | 6:Y:59:ALA:N     | 2.85                     | 0.49              |
| 6:Y:133:ARG:HG3   | 6:Y:137:ARG:HE   | 1.77                     | 0.49              |
| 1:e:205:MET:HE1   | 1:e:249:LYS:HD3  | 1.94                     | 0.49              |
| 1:f:73:LEU:HD22   | 1:f:238:ARG:HH21 | 1.77                     | 0.49              |
| 1:f:142:ASN:HA    | 1:f:370:LEU:HG   | 1.95                     | 0.49              |
| 2:A:145:VAL:HA    | 2:A:150:ILE:HG22 | 1.94                     | 0.49              |
| 2:A:447:LYS:HE3   | 2:A:471:GLU:N    | 2.28                     | 0.49              |
| 3:U:257:VAL:HA    | 3:U:260:LEU:HD13 | 1.94                     | 0.49              |
| 3:V:104:LYS:HD3   | 3:V:110:VAL:HG22 | 1.95                     | 0.49              |
| 5:X:1122:LYS:HG2  | 5:X:1229:TYR:CE1 | 2.48                     | 0.49              |
| 6:Y:865:HIS:H     | 6:Y:868:TRP:HD1  | 1.60                     | 0.49              |
| 1:e:401:ASN:O     | 1:e:405:MET:HG2  | 2.12                     | 0.49              |
| 1:e:409:ASN:OD1   | 1:e:409:ASN:N    | 2.41                     | 0.49              |
| 1:f:156:ASP:O     | 1:f:157:LEU:C    | 2.54                     | 0.49              |
| 2:A:163:LEU:O     | 2:A:167:MET:HG3  | 2.13                     | 0.49              |
| 5:X:448:LEU:HD21  | 5:X:587:LEU:HD12 | 1.95                     | 0.49              |
| 1:d:401:ASN:O     | 1:d:405:MET:HG2  | 2.12                     | 0.49              |
| 3:U:25:LYS:HE3    | 3:U:204:GLU:HB3  | 1.93                     | 0.49              |
| 6:Y:210:SER:OG    | 6:Y:211:GLU:N    | 2.46                     | 0.49              |
| 1:a:106:GLU:OE1   | 1:a:106:GLU:N    | 2.35                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:142:ASN:HA    | 1:a:370:LEU:HG    | 1.95                     | 0.49              |
| 1:b:73:LEU:HD22   | 1:b:238:ARG:HH21  | 1.77                     | 0.49              |
| 1:b:330:VAL:O     | 1:b:334:GLU:HG2   | 2.13                     | 0.49              |
| 1:c:10:PRO:HG2    | 1:c:13:GLU:HB2    | 1.94                     | 0.49              |
| 1:c:142:ASN:HA    | 1:c:370:LEU:HG    | 1.95                     | 0.49              |
| 1:f:59:GLN:OE1    | 1:f:59:GLN:N      | 2.27                     | 0.49              |
| 2:A:441:ASP:H     | 2:A:444:LEU:HD13  | 1.78                     | 0.49              |
| 3:U:302:GLU:O     | 3:U:306:VAL:HG22  | 2.12                     | 0.49              |
| 3:V:81:ILE:HG12   | 3:V:131:CYS:SG    | 2.52                     | 0.49              |
| 5:X:646:SER:OG    | 5:X:648:ASP:OD1   | 2.27                     | 0.49              |
| 6:Y:460:ASP:N     | 6:Y:460:ASP:OD1   | 2.45                     | 0.49              |
| 6:Y:1221:LEU:HD22 | 6:Y:1306:LEU:HG   | 1.93                     | 0.49              |
| 1:e:10:PRO:HG2    | 1:e:13:GLU:HB2    | 1.94                     | 0.49              |
| 3:U:195:ARG:HD2   | 3:U:198:LEU:HD11  | 1.95                     | 0.49              |
| 5:X:1102:GLY:HA3  | 5:X:1106:ARG:HH11 | 1.78                     | 0.49              |
| 6:Y:814:CYS:SG    | 6:Y:883:ARG:NH1   | 2.86                     | 0.49              |
| 1:b:3:LEU:HD12    | 1:b:7:LYS:HE2     | 1.93                     | 0.48              |
| 1:d:179:PRO:O     | 1:d:184:LYS:NZ    | 2.45                     | 0.48              |
| 1:d:406:THR:OG1   | 1:d:411:ASP:HB3   | 2.13                     | 0.48              |
| 3:V:105:SER:OG    | 3:V:106:GLY:N     | 2.45                     | 0.48              |
| 6:Y:944:ALA:HB1   | 6:Y:947:GLU:HB2   | 1.95                     | 0.48              |
| 6:Y:1155:ILE:HD13 | 6:Y:1194:ARG:HH22 | 1.78                     | 0.48              |
| 1:b:406:THR:OG1   | 1:b:411:ASP:HB3   | 2.13                     | 0.48              |
| 1:c:205:MET:HE1   | 1:c:249:LYS:HD3   | 1.94                     | 0.48              |
| 1:c:406:THR:OG1   | 1:c:411:ASP:HB3   | 2.13                     | 0.48              |
| 5:X:699:LEU:HD23  | 5:X:799:ASN:CG    | 2.38                     | 0.48              |
| 5:X:807:TRP:HB2   | 5:X:1097:VAL:HG11 | 1.94                     | 0.48              |
| 5:X:1117:LEU:HD13 | 5:X:1195:ILE:HG12 | 1.95                     | 0.48              |
| 6:Y:160:LEU:HD22  | 6:Y:164:GLN:HB3   | 1.95                     | 0.48              |
| 6:Y:226:ALA:O     | 6:Y:230:SER:OG    | 2.31                     | 0.48              |
| 6:Y:417:ARG:HG2   | 6:Y:418:GLU:HG2   | 1.95                     | 0.48              |
| 8:L:6:DC:H2'      | 8:L:7:DA:H8       | 1.78                     | 0.48              |
| 1:f:18:GLY:HA3    | 1:f:26:LEU:HD13   | 1.96                     | 0.48              |
| 2:A:113:VAL:O     | 2:A:116:GLN:HG3   | 2.13                     | 0.48              |
| 5:X:1126:ASP:HA   | 5:X:1129:ASN:HD21 | 1.78                     | 0.48              |
| 1:a:295:HIS:HE1   | 1:a:299:ARG:HH21  | 1.61                     | 0.48              |
| 1:a:330:VAL:O     | 1:a:334:GLU:HG2   | 2.13                     | 0.48              |
| 1:b:176:ILE:HB    | 1:b:318:THR:HG23  | 1.96                     | 0.48              |
| 1:b:247:ILE:HB    | 1:b:300:PHE:HE1   | 1.77                     | 0.48              |
| 1:c:295:HIS:HE1   | 1:c:299:ARG:HH21  | 1.61                     | 0.48              |
| 1:c:401:ASN:O     | 1:c:405:MET:HG2   | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:d:31:LYS:HG3   | 1:d:32:GLN:N     | 2.29                     | 0.48              |
| 2:A:91:ASP:OD1   | 2:A:91:ASP:N     | 2.43                     | 0.48              |
| 2:A:441:ASP:HB2  | 2:A:444:LEU:HD13 | 1.94                     | 0.48              |
| 4:W:43:ASN:O     | 6:Y:417:ARG:NE   | 2.46                     | 0.48              |
| 5:X:35:PHE:CD2   | 5:X:130:MET:HG2  | 2.48                     | 0.48              |
| 5:X:361:SER:HA   | 5:X:364:VAL:HG22 | 1.95                     | 0.48              |
| 6:Y:156:ARG:NH2  | 6:Y:191:SER:OG   | 2.46                     | 0.48              |
| 8:L:-1:DA:H2'    | 8:L:0:DA:C8      | 2.48                     | 0.48              |
| 8:L:9:DG:H2''    | 8:L:10:DC:H5'    | 1.96                     | 0.48              |
| 1:a:31:LYS:HG3   | 1:a:32:GLN:N     | 2.29                     | 0.48              |
| 1:b:106:GLU:OE1  | 1:b:106:GLU:N    | 2.35                     | 0.48              |
| 1:c:176:ILE:HB   | 1:c:318:THR:HG23 | 1.96                     | 0.48              |
| 1:f:176:ILE:HB   | 1:f:318:THR:HG23 | 1.96                     | 0.48              |
| 3:U:61:ILE:HB    | 3:U:64:VAL:HG12  | 1.96                     | 0.48              |
| 5:X:812:PHE:CD2  | 5:X:813:GLU:HG2  | 2.48                     | 0.48              |
| 5:X:1331:ARG:NH2 | 5:X:1337:ILE:O   | 2.47                     | 0.48              |
| 6:Y:269:TYR:CD1  | 6:Y:306:LEU:HD11 | 2.49                     | 0.48              |
| 6:Y:966:VAL:HG11 | 6:Y:1030:GLU:HA  | 1.94                     | 0.48              |
| 1:b:205:MET:HE1  | 1:b:249:LYS:HD3  | 1.94                     | 0.48              |
| 1:d:176:ILE:HB   | 1:d:318:THR:HG23 | 1.96                     | 0.48              |
| 1:e:142:ASN:HA   | 1:e:370:LEU:HG   | 1.95                     | 0.48              |
| 1:e:388:HIS:HE1  | 1:f:351:GLU:OE1  | 1.96                     | 0.48              |
| 1:f:330:VAL:O    | 1:f:334:GLU:HG2  | 2.13                     | 0.48              |
| 5:X:801:ARG:HG2  | 5:X:1229:TYR:CE1 | 2.48                     | 0.48              |
| 5:X:976:ARG:HB2  | 5:X:994:ARG:NH2  | 2.29                     | 0.48              |
| 6:Y:962:ASN:HB3  | 6:Y:964:LYS:HZ1  | 1.77                     | 0.48              |
| 1:a:406:THR:OG1  | 1:a:411:ASP:HB3  | 2.13                     | 0.48              |
| 1:e:406:THR:OG1  | 1:e:411:ASP:HB3  | 2.13                     | 0.48              |
| 2:A:22:LYS:C     | 2:A:117:LYS:HZ1  | 2.21                     | 0.48              |
| 5:X:516:ASP:N    | 5:X:516:ASP:OD1  | 2.47                     | 0.48              |
| 5:X:883:LEU:HD21 | 5:X:918:LEU:HD23 | 1.94                     | 0.48              |
| 6:Y:390:LEU:HD21 | 6:Y:400:MET:HE1  | 1.94                     | 0.48              |
| 1:b:18:GLY:HA3   | 1:b:26:LEU:HD13  | 1.96                     | 0.48              |
| 1:c:73:LEU:HD13  | 1:c:238:ARG:HH21 | 1.79                     | 0.48              |
| 1:c:330:VAL:O    | 1:c:334:GLU:HG2  | 2.13                     | 0.48              |
| 1:f:10:PRO:HG2   | 1:f:13:GLU:HB2   | 1.94                     | 0.48              |
| 2:A:213:VAL:HB   | 2:A:216:ILE:HG22 | 1.95                     | 0.48              |
| 4:W:44:ASP:HB2   | 6:Y:418:GLU:HG3  | 1.95                     | 0.48              |
| 5:X:796:LEU:HB3  | 5:X:1233:LEU:CD2 | 2.43                     | 0.48              |
| 6:Y:381:ILE:HD11 | 6:Y:412:LEU:HD13 | 1.95                     | 0.48              |
| 1:a:18:GLY:HA3   | 1:a:26:LEU:HD13  | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:28:ARG:NH2    | 2:A:177:ASP:HB3   | 2.28                     | 0.48              |
| 1:b:184:LYS:H     | 11:b:502:ADP:PB   | 2.37                     | 0.48              |
| 1:f:406:THR:OG1   | 1:f:411:ASP:HB3   | 2.13                     | 0.48              |
| 5:X:701:GLY:N     | 5:X:1182:ILE:O    | 2.47                     | 0.48              |
| 6:Y:1305:ASP:OD1  | 6:Y:1305:ASP:N    | 2.47                     | 0.48              |
| 1:b:388:HIS:HE1   | 1:c:351:GLU:CD    | 2.21                     | 0.48              |
| 1:c:274:TYR:HD2   | 1:c:297:PRO:HG3   | 1.79                     | 0.48              |
| 1:d:73:LEU:HD13   | 1:d:238:ARG:HH21  | 1.79                     | 0.48              |
| 1:d:142:ASN:HA    | 1:d:370:LEU:HG    | 1.95                     | 0.48              |
| 1:d:330:VAL:O     | 1:d:334:GLU:HG2   | 2.13                     | 0.48              |
| 1:e:330:VAL:O     | 1:e:334:GLU:HG2   | 2.13                     | 0.48              |
| 2:A:109:THR:O     | 2:A:112:GLN:HG3   | 2.14                     | 0.48              |
| 2:A:479:GLY:HA2   | 2:A:482:ILE:HG22  | 1.96                     | 0.48              |
| 2:A:487:ASN:HA    | 2:A:491:PHE:HB3   | 1.96                     | 0.48              |
| 5:X:376:PRO:HB3   | 5:X:380:ALA:HB3   | 1.96                     | 0.48              |
| 7:K:-13:DA:H2"    | 7:K:-12:DG:C8     | 2.48                     | 0.48              |
| 1:a:31:LYS:HB2    | 1:a:31:LYS:HE2    | 1.45                     | 0.47              |
| 1:b:73:LEU:HD13   | 1:b:238:ARG:HH21  | 1.79                     | 0.47              |
| 1:b:173:ARG:HD3   | 1:b:301:PHE:O     | 2.14                     | 0.47              |
| 1:c:31:LYS:HG3    | 1:c:32:GLN:N      | 2.29                     | 0.47              |
| 1:e:18:GLY:HA3    | 1:e:26:LEU:HD13   | 1.96                     | 0.47              |
| 1:e:178:ALA:HB2   | 1:e:345:LEU:HB2   | 1.96                     | 0.47              |
| 5:X:318:SER:OG    | 5:X:319:LEU:N     | 2.47                     | 0.47              |
| 5:X:810:TYR:O     | 5:X:815:SER:OG    | 2.32                     | 0.47              |
| 5:X:1119:MET:HG2  | 5:X:1204:LEU:HD13 | 1.96                     | 0.47              |
| 5:X:1253:LEU:HD11 | 6:Y:251:PRO:HG3   | 1.94                     | 0.47              |
| 1:d:18:GLY:HA3    | 1:d:26:LEU:HD13   | 1.96                     | 0.47              |
| 1:d:178:ALA:HB2   | 1:d:345:LEU:HB2   | 1.96                     | 0.47              |
| 1:d:295:HIS:HE1   | 1:d:299:ARG:HH21  | 1.61                     | 0.47              |
| 1:f:274:TYR:HD2   | 1:f:297:PRO:HG3   | 1.79                     | 0.47              |
| 3:U:303:ILE:O     | 3:U:307:LEU:HB2   | 2.13                     | 0.47              |
| 3:V:182:ARG:HG2   | 3:V:206:GLU:HB3   | 1.96                     | 0.47              |
| 5:X:1064:ASP:HB2  | 5:X:1076:ILE:HD13 | 1.96                     | 0.47              |
| 6:Y:406:ALA:HA    | 6:Y:409:TRP:HD1   | 1.79                     | 0.47              |
| 6:Y:430:HIS:CD2   | 6:Y:432:LEU:HB3   | 2.49                     | 0.47              |
| 2:A:137:ILE:HA    | 2:A:181:GLY:O     | 2.14                     | 0.47              |
| 5:X:425:ILE:HA    | 5:X:428:VAL:HG12  | 1.95                     | 0.47              |
| 1:b:31:LYS:HG3    | 1:b:32:GLN:N      | 2.29                     | 0.47              |
| 2:A:26:ALA:HB2    | 2:A:117:LYS:CD    | 2.41                     | 0.47              |
| 2:A:127:VAL:HG21  | 2:A:187:ARG:O     | 2.13                     | 0.47              |
| 2:A:307:ILE:HB    | 2:A:336:LEU:HD23  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:X:300:ASP:OD1  | 5:X:313:ALA:N     | 2.48                     | 0.47              |
| 6:Y:129:ASP:HB2  | 6:Y:220:ARG:HH12  | 1.80                     | 0.47              |
| 6:Y:355:ILE:HD11 | 6:Y:466:MET:HG3   | 1.96                     | 0.47              |
| 6:Y:620:PHE:CZ   | 6:Y:624:ILE:HD11  | 2.48                     | 0.47              |
| 1:c:18:GLY:HA3   | 1:c:26:LEU:HD13   | 1.95                     | 0.47              |
| 1:c:148:GLU:HB3  | 1:c:160:ARG:HG2   | 1.97                     | 0.47              |
| 1:c:173:ARG:HD3  | 1:c:301:PHE:O     | 2.14                     | 0.47              |
| 1:d:173:ARG:HD3  | 1:d:301:PHE:O     | 2.14                     | 0.47              |
| 1:d:375:GLU:OE2  | 1:d:375:GLU:N     | 2.48                     | 0.47              |
| 1:e:73:LEU:HD13  | 1:e:238:ARG:HH21  | 1.79                     | 0.47              |
| 1:f:31:LYS:HG3   | 1:f:32:GLN:N      | 2.29                     | 0.47              |
| 6:Y:968:ASN:ND2  | 6:Y:970:SER:OG    | 2.48                     | 0.47              |
| 1:b:142:ASN:HA   | 1:b:370:LEU:HG    | 1.95                     | 0.47              |
| 1:c:247:ILE:HB   | 1:c:300:PHE:HE1   | 1.77                     | 0.47              |
| 1:c:375:GLU:OE2  | 1:c:375:GLU:N     | 2.48                     | 0.47              |
| 1:d:148:GLU:HB3  | 1:d:160:ARG:HG2   | 1.97                     | 0.47              |
| 1:e:31:LYS:HG3   | 1:e:32:GLN:N      | 2.29                     | 0.47              |
| 1:e:383:LEU:HD13 | 1:e:383:LEU:HA    | 1.69                     | 0.47              |
| 1:f:173:ARG:HD3  | 1:f:301:PHE:O     | 2.14                     | 0.47              |
| 1:f:375:GLU:OE2  | 1:f:375:GLU:N     | 2.48                     | 0.47              |
| 5:X:105:TYR:HB2  | 5:X:114:VAL:HG23  | 1.97                     | 0.47              |
| 5:X:1321:GLU:O   | 5:X:1325:VAL:HG23 | 2.15                     | 0.47              |
| 6:Y:19:ALA:HA    | 6:Y:1344:LEU:HD22 | 1.95                     | 0.47              |
| 1:a:173:ARG:HD3  | 1:a:301:PHE:O     | 2.14                     | 0.47              |
| 1:b:178:ALA:HB2  | 1:b:345:LEU:HB2   | 1.96                     | 0.47              |
| 1:b:274:TYR:HD2  | 1:b:297:PRO:HG3   | 1.79                     | 0.47              |
| 1:e:176:ILE:HB   | 1:e:318:THR:HG23  | 1.96                     | 0.47              |
| 1:e:375:GLU:OE2  | 1:e:375:GLU:N     | 2.48                     | 0.47              |
| 1:f:295:HIS:HE1  | 1:f:299:ARG:HH21  | 1.61                     | 0.47              |
| 5:X:551:HIS:HB3  | 5:X:553:THR:HG22  | 1.96                     | 0.47              |
| 5:X:700:VAL:HG21 | 5:X:1114:GLU:HG3  | 1.97                     | 0.47              |
| 5:X:1326:LEU:O   | 5:X:1330:ILE:HG12 | 2.15                     | 0.47              |
| 6:Y:1111:ASP:OD1 | 6:Y:1112:GLY:N    | 2.48                     | 0.47              |
| 6:Y:1184:ASP:OD1 | 6:Y:1184:ASP:N    | 2.47                     | 0.47              |
| 1:b:148:GLU:HB3  | 1:b:160:ARG:HG2   | 1.97                     | 0.47              |
| 1:c:161:VAL:HG13 | 1:c:399:LEU:HD21  | 1.97                     | 0.47              |
| 1:c:264:LEU:HD21 | 1:c:270:LEU:HD21  | 1.97                     | 0.47              |
| 1:e:274:TYR:HD2  | 1:e:297:PRO:HG3   | 1.79                     | 0.47              |
| 1:f:73:LEU:HD13  | 1:f:238:ARG:HH21  | 1.79                     | 0.47              |
| 1:f:247:ILE:HB   | 1:f:300:PHE:HE1   | 1.77                     | 0.47              |
| 1:f:264:LEU:HD21 | 1:f:270:LEU:HD21  | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:X:668:ILE:HB   | 5:X:671:LEU:HD13 | 1.97                     | 0.47              |
| 5:X:1006:GLU:OE2 | 5:X:1007:LYS:HG2 | 2.15                     | 0.47              |
| 6:Y:697:MET:HE3  | 6:Y:697:MET:HB3  | 1.83                     | 0.47              |
| 1:b:134:GLU:OE1  | 1:b:134:GLU:N    | 2.47                     | 0.47              |
| 1:b:375:GLU:OE2  | 1:b:375:GLU:N    | 2.48                     | 0.47              |
| 1:e:173:ARG:HD3  | 1:e:301:PHE:O    | 2.14                     | 0.47              |
| 1:f:161:VAL:HG13 | 1:f:399:LEU:HD21 | 1.97                     | 0.47              |
| 6:Y:576:ARG:HD3  | 6:Y:593:ASN:HA   | 1.97                     | 0.47              |
| 1:a:83:PRO:HD2   | 8:L:19:DG:H2"    | 1.96                     | 0.47              |
| 1:a:375:GLU:OE2  | 1:a:375:GLU:N    | 2.48                     | 0.47              |
| 1:b:264:LEU:HD21 | 1:b:270:LEU:HD21 | 1.97                     | 0.47              |
| 1:c:178:ALA:HB2  | 1:c:345:LEU:HB2  | 1.96                     | 0.47              |
| 1:f:178:ALA:HB2  | 1:f:345:LEU:HB2  | 1.96                     | 0.47              |
| 2:A:213:VAL:HG12 | 2:A:215:GLU:H    | 1.80                     | 0.47              |
| 4:W:7:GLN:OE1    | 4:W:16:ARG:NH1   | 2.48                     | 0.47              |
| 8:L:11:DG:H2"    | 8:L:12:DC:C5     | 2.49                     | 0.47              |
| 1:a:148:GLU:HB3  | 1:a:160:ARG:HG2  | 1.97                     | 0.46              |
| 1:a:247:ILE:HB   | 1:a:300:PHE:HE1  | 1.77                     | 0.46              |
| 1:b:161:VAL:HG13 | 1:b:399:LEU:HD21 | 1.97                     | 0.46              |
| 1:e:157:LEU:O    | 1:e:161:VAL:HG23 | 2.16                     | 0.46              |
| 1:e:161:VAL:HG13 | 1:e:399:LEU:HD21 | 1.97                     | 0.46              |
| 5:X:36:GLN:O     | 5:X:40:GLU:HG2   | 2.15                     | 0.46              |
| 6:Y:332:LYS:HG2  | 6:Y:1328:THR:HB  | 1.97                     | 0.46              |
| 1:a:73:LEU:HD13  | 1:a:238:ARG:HH21 | 1.79                     | 0.46              |
| 1:b:157:LEU:O    | 1:b:161:VAL:HG23 | 2.16                     | 0.46              |
| 1:c:157:LEU:O    | 1:c:161:VAL:HG23 | 2.16                     | 0.46              |
| 1:d:264:LEU:HD21 | 1:d:270:LEU:HD21 | 1.97                     | 0.46              |
| 1:e:247:ILE:HB   | 1:e:300:PHE:HE1  | 1.77                     | 0.46              |
| 2:A:103:ASP:O    | 2:A:106:THR:OG1  | 2.27                     | 0.46              |
| 3:U:239:GLN:HG3  | 3:V:12:ARG:HD3   | 1.97                     | 0.46              |
| 5:X:557:ARG:HH22 | 5:X:611:GLU:CD   | 2.21                     | 0.46              |
| 1:b:120:ASN:HB2  | 1:b:256:HIS:CE1  | 2.51                     | 0.46              |
| 1:c:266:SER:OG   | 1:c:267:ILE:N    | 2.49                     | 0.46              |
| 1:e:179:PRO:O    | 1:e:184:LYS:NZ   | 2.45                     | 0.46              |
| 2:A:67:GLU:HG3   | 2:A:74:GLU:OE1   | 2.15                     | 0.46              |
| 5:X:161:LYS:HB3  | 5:X:170:VAL:HG23 | 1.97                     | 0.46              |
| 5:X:241:LEU:HD22 | 5:X:285:ILE:HD13 | 1.96                     | 0.46              |
| 5:X:1282:GLY:HA2 | 6:Y:1360:GLY:HA3 | 1.97                     | 0.46              |
| 1:a:157:LEU:O    | 1:a:161:VAL:HG23 | 2.16                     | 0.46              |
| 1:d:157:LEU:O    | 1:d:161:VAL:HG23 | 2.16                     | 0.46              |
| 1:e:174:GLY:HA2  | 1:e:341:MET:HB3  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:f:120:ASN:HB2  | 1:f:256:HIS:CE1  | 2.51                     | 0.46              |
| 1:f:157:LEU:O    | 1:f:161:VAL:HG23 | 2.16                     | 0.46              |
| 1:f:265:ASP:HA   | 1:f:266:SER:HA   | 1.49                     | 0.46              |
| 2:A:344:LEU:HB3  | 2:A:350:ALA:HB2  | 1.97                     | 0.46              |
| 5:X:11:ILE:HG23  | 5:X:1149:TYR:CZ  | 2.50                     | 0.46              |
| 5:X:538:LEU:HD23 | 5:X:538:LEU:H    | 1.81                     | 0.46              |
| 6:Y:423:LEU:HD23 | 6:Y:437:PHE:HB2  | 1.97                     | 0.46              |
| 7:K:2:DG:H2'     | 7:K:3:DT:H71     | 1.97                     | 0.46              |
| 8:L:6:DC:H2'     | 8:L:7:DA:C8      | 2.50                     | 0.46              |
| 1:a:178:ALA:HB2  | 1:a:345:LEU:HB2  | 1.96                     | 0.46              |
| 1:a:266:SER:OG   | 1:a:267:ILE:N    | 2.49                     | 0.46              |
| 1:a:348:LYS:HE3  | 1:a:393:ILE:HD11 | 1.98                     | 0.46              |
| 1:b:383:LEU:HD13 | 1:b:383:LEU:HA   | 1.69                     | 0.46              |
| 1:e:295:HIS:HE1  | 1:e:299:ARG:HH21 | 1.61                     | 0.46              |
| 1:f:174:GLY:HA2  | 1:f:341:MET:HB3  | 1.98                     | 0.46              |
| 6:Y:84:ILE:HB    | 6:Y:89:GLY:HA2   | 1.97                     | 0.46              |
| 6:Y:377:PHE:HD2  | 6:Y:380:PHE:HD2  | 1.64                     | 0.46              |
| 1:a:161:VAL:HG13 | 1:a:399:LEU:HD21 | 1.97                     | 0.46              |
| 1:d:266:SER:OG   | 1:d:267:ILE:N    | 2.49                     | 0.46              |
| 1:f:348:LYS:HE3  | 1:f:393:ILE:HD11 | 1.98                     | 0.46              |
| 3:V:61:ILE:HB    | 3:V:64:VAL:HG12  | 1.96                     | 0.46              |
| 5:X:513:GLN:HE21 | 5:X:526:HIS:CE1  | 2.34                     | 0.46              |
| 5:X:672:GLU:HG3  | 6:Y:766:GLY:HA2  | 1.98                     | 0.46              |
| 5:X:1283:ALA:HA  | 6:Y:479:GLU:HG2  | 1.96                     | 0.46              |
| 1:a:176:ILE:HB   | 1:a:318:THR:HG23 | 1.96                     | 0.46              |
| 1:b:295:HIS:HE1  | 1:b:299:ARG:HH21 | 1.61                     | 0.46              |
| 1:c:31:LYS:HB2   | 1:c:31:LYS:HE2   | 1.45                     | 0.46              |
| 1:d:171:GLY:N    | 1:d:314:THR:HG1  | 2.13                     | 0.46              |
| 2:A:23:ILE:HG22  | 2:A:51:ARG:NH1   | 2.31                     | 0.46              |
| 2:A:444:LEU:HD12 | 2:A:444:LEU:H    | 1.81                     | 0.46              |
| 3:U:9:LEU:HD11   | 3:U:30:PRO:HG2   | 1.96                     | 0.46              |
| 5:X:596:ASP:OD1  | 5:X:596:ASP:N    | 2.49                     | 0.46              |
| 6:Y:982:LEU:HD11 | 6:Y:995:TYR:HD2  | 1.81                     | 0.46              |
| 6:Y:1084:GLN:OE1 | 6:Y:1086:ASN:N   | 2.49                     | 0.46              |
| 1:a:59:GLN:OE1   | 1:a:59:GLN:N     | 2.27                     | 0.46              |
| 1:a:120:ASN:HB2  | 1:a:256:HIS:CE1  | 2.51                     | 0.46              |
| 1:d:337:GLY:O    | 1:e:212:ARG:NH2  | 2.49                     | 0.46              |
| 1:e:348:LYS:HE3  | 1:e:393:ILE:HD11 | 1.98                     | 0.46              |
| 1:f:75:GLY:N     | 1:f:78:ASP:OD2   | 2.47                     | 0.46              |
| 2:A:152:LEU:HD13 | 2:A:162:ILE:HG13 | 1.97                     | 0.46              |
| 5:X:230:PHE:CZ   | 5:X:292:ILE:HD13 | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:X:735:LYS:HA   | 5:X:748:ILE:HG22 | 1.98                     | 0.46              |
| 6:Y:116:PHE:O    | 6:Y:122:SER:OG   | 2.30                     | 0.46              |
| 1:a:264:LEU:HD21 | 1:a:270:LEU:HD21 | 1.97                     | 0.46              |
| 1:c:348:LYS:HE3  | 1:c:393:ILE:HD11 | 1.98                     | 0.46              |
| 1:d:161:VAL:HG13 | 1:d:399:LEU:HD21 | 1.97                     | 0.46              |
| 1:e:148:GLU:HB3  | 1:e:160:ARG:HG2  | 1.97                     | 0.46              |
| 2:A:348:HIS:CD2  | 2:A:349:GLN:HG2  | 2.51                     | 0.46              |
| 2:A:413:ALA:HA   | 2:A:416:THR:HG22 | 1.97                     | 0.46              |
| 2:A:447:LYS:HE3  | 2:A:470:ILE:HA   | 1.98                     | 0.46              |
| 5:X:233:ARG:HG3  | 5:X:238:GLN:HB2  | 1.97                     | 0.46              |
| 5:X:891:GLY:N    | 5:X:911:SER:HB3  | 2.30                     | 0.46              |
| 6:Y:263:SER:OG   | 6:Y:266:ASN:OD1  | 2.33                     | 0.46              |
| 6:Y:968:ASN:OD1  | 6:Y:972:LYS:N    | 2.48                     | 0.46              |
| 1:b:348:LYS:HE3  | 1:b:393:ILE:HD11 | 1.98                     | 0.46              |
| 1:c:120:ASN:HB2  | 1:c:256:HIS:CE1  | 2.51                     | 0.46              |
| 1:d:383:LEU:HD13 | 1:d:383:LEU:HA   | 1.69                     | 0.46              |
| 1:e:264:LEU:HD21 | 1:e:270:LEU:HD21 | 1.97                     | 0.46              |
| 1:f:382:ILE:HG13 | 1:f:383:LEU:N    | 2.31                     | 0.46              |
| 2:A:124:ALA:HA   | 2:A:127:VAL:HG12 | 1.98                     | 0.46              |
| 2:A:184:TYR:CZ   | 2:A:196:PHE:HB3  | 2.50                     | 0.46              |
| 5:X:320:ASP:OD1  | 5:X:320:ASP:N    | 2.49                     | 0.46              |
| 6:Y:576:ARG:NH1  | 6:Y:592:VAL:O    | 2.49                     | 0.46              |
| 1:a:274:TYR:HD2  | 1:a:297:PRO:HG3  | 1.79                     | 0.45              |
| 1:c:174:GLY:HA2  | 1:c:341:MET:HB3  | 1.98                     | 0.45              |
| 1:d:166:SER:HB2  | 1:d:341:MET:HE1  | 1.98                     | 0.45              |
| 1:d:274:TYR:HD2  | 1:d:297:PRO:HG3  | 1.79                     | 0.45              |
| 1:e:266:SER:OG   | 1:e:267:ILE:N    | 2.49                     | 0.45              |
| 2:A:47:VAL:HG22  | 2:A:56:PHE:HB2   | 1.98                     | 0.45              |
| 5:X:448:LEU:H    | 5:X:553:THR:HG21 | 1.81                     | 0.45              |
| 1:a:234:GLU:HB2  | 1:a:238:ARG:HB2  | 1.99                     | 0.45              |
| 1:d:309:GLU:H    | 1:d:309:GLU:HG2  | 1.52                     | 0.45              |
| 1:d:382:ILE:HG13 | 1:d:383:LEU:N    | 2.31                     | 0.45              |
| 1:e:120:ASN:HB2  | 1:e:256:HIS:CE1  | 2.51                     | 0.45              |
| 1:f:148:GLU:HB3  | 1:f:160:ARG:HG2  | 1.97                     | 0.45              |
| 3:V:220:ALA:O    | 3:V:223:ILE:HG22 | 2.16                     | 0.45              |
| 5:X:149:LEU:HD11 | 5:X:451:ARG:HB3  | 1.97                     | 0.45              |
| 6:Y:431:ARG:HD3  | 6:Y:493:PRO:HG3  | 1.98                     | 0.45              |
| 6:Y:533:ALA:HB1  | 6:Y:574:VAL:HG13 | 1.99                     | 0.45              |
| 1:a:134:GLU:OE1  | 1:a:134:GLU:N    | 2.47                     | 0.45              |
| 1:c:166:SER:HB2  | 1:c:341:MET:HE1  | 1.98                     | 0.45              |
| 1:d:247:ILE:HB   | 1:d:300:PHE:HE1  | 1.77                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:e:56:GLU:HA    | 1:e:93:THR:HG22  | 1.99                     | 0.45              |
| 1:e:114:LEU:HA   | 2:A:84:ASP:HB2   | 1.97                     | 0.45              |
| 5:X:593:LYS:O    | 5:X:600:THR:OG1  | 2.28                     | 0.45              |
| 8:L:4:DC:H2'     | 8:L:5:DA:C8      | 2.50                     | 0.45              |
| 1:a:27:ALA:HB3   | 1:a:28:ARG:HH12  | 1.82                     | 0.45              |
| 1:b:91:LEU:HD13  | 1:b:97:ILE:HD11  | 1.99                     | 0.45              |
| 1:b:124:PRO:O    | 1:b:127:ALA:HB3  | 2.17                     | 0.45              |
| 1:c:171:GLY:N    | 1:c:314:THR:OG1  | 2.38                     | 0.45              |
| 1:c:309:GLU:H    | 1:c:309:GLU:HG2  | 1.52                     | 0.45              |
| 1:d:124:PRO:O    | 1:d:127:ALA:HB3  | 2.17                     | 0.45              |
| 1:d:262:ILE:HB   | 1:d:315:ILE:HG22 | 1.99                     | 0.45              |
| 1:e:166:SER:HB2  | 1:e:341:MET:HE1  | 1.98                     | 0.45              |
| 1:e:171:GLY:N    | 1:e:314:THR:OG1  | 2.38                     | 0.45              |
| 2:A:252:VAL:O    | 2:A:258:ARG:N    | 2.46                     | 0.45              |
| 4:W:7:GLN:HB2    | 6:Y:614:LEU:HD23 | 1.96                     | 0.45              |
| 5:X:797:GLY:N    | 5:X:1231:TYR:OH  | 2.46                     | 0.45              |
| 6:Y:697:MET:HE2  | 6:Y:738:ARG:HA   | 1.99                     | 0.45              |
| 6:Y:1183:SER:OG  | 6:Y:1184:ASP:N   | 2.48                     | 0.45              |
| 1:a:124:PRO:O    | 1:a:127:ALA:HB3  | 2.17                     | 0.45              |
| 1:a:174:GLY:HA2  | 1:a:341:MET:HB3  | 1.97                     | 0.45              |
| 1:b:179:PRO:O    | 1:b:184:LYS:NZ   | 2.45                     | 0.45              |
| 1:b:184:LYS:N    | 11:b:502:ADP:O3B | 2.49                     | 0.45              |
| 5:X:187:GLU:O    | 5:X:194:LEU:HD12 | 2.17                     | 0.45              |
| 6:Y:131:PRO:HG2  | 6:Y:134:ASP:OD2  | 2.17                     | 0.45              |
| 6:Y:410:ASP:OD1  | 6:Y:411:ILE:N    | 2.49                     | 0.45              |
| 6:Y:576:ARG:NH1  | 6:Y:594:GLN:H    | 2.14                     | 0.45              |
| 1:a:166:SER:HB2  | 1:a:341:MET:HE1  | 1.98                     | 0.45              |
| 1:b:234:GLU:HB2  | 1:b:238:ARG:HB2  | 1.98                     | 0.45              |
| 1:b:382:ILE:HG13 | 1:b:383:LEU:N    | 2.31                     | 0.45              |
| 1:c:56:GLU:HA    | 1:c:93:THR:HG22  | 1.99                     | 0.45              |
| 1:e:124:PRO:O    | 1:e:127:ALA:HB3  | 2.17                     | 0.45              |
| 1:e:134:GLU:OE1  | 1:e:134:GLU:N    | 2.47                     | 0.45              |
| 1:f:56:GLU:HA    | 1:f:93:THR:HG22  | 1.99                     | 0.45              |
| 5:X:1070:HIS:CG  | 5:X:1111:GLN:HB3 | 2.52                     | 0.45              |
| 6:Y:105:ILE:HB   | 6:Y:242:LEU:HB2  | 1.98                     | 0.45              |
| 1:b:31:LYS:HE2   | 1:b:31:LYS:HB2   | 1.45                     | 0.45              |
| 1:b:174:GLY:HA2  | 1:b:341:MET:HB3  | 1.98                     | 0.45              |
| 1:b:262:ILE:HB   | 1:b:315:ILE:HG22 | 1.99                     | 0.45              |
| 1:c:382:ILE:HG13 | 1:c:383:LEU:N    | 2.31                     | 0.45              |
| 1:d:56:GLU:HA    | 1:d:93:THR:HG22  | 1.99                     | 0.45              |
| 1:d:91:LEU:HD13  | 1:d:97:ILE:HD11  | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:d:120:ASN:HB2   | 1:d:256:HIS:CE1   | 2.51                     | 0.45              |
| 1:d:171:GLY:N     | 1:d:314:THR:OG1   | 2.38                     | 0.45              |
| 1:d:174:GLY:HA2   | 1:d:341:MET:HB3   | 1.98                     | 0.45              |
| 1:e:265:ASP:HA    | 1:e:266:SER:HA    | 1.49                     | 0.45              |
| 5:X:1009:ASN:O    | 5:X:1012:GLU:HG3  | 2.15                     | 0.45              |
| 6:Y:147:ILE:HB    | 6:Y:148:GLU:OE2   | 2.17                     | 0.45              |
| 1:b:266:SER:OG    | 1:b:267:ILE:N     | 2.49                     | 0.45              |
| 1:c:130:LYS:HG2   | 1:d:28:ARG:NH2    | 2.32                     | 0.45              |
| 1:d:348:LYS:HE3   | 1:d:393:ILE:HD11  | 1.98                     | 0.45              |
| 1:f:234:GLU:HB2   | 1:f:238:ARG:HB2   | 1.98                     | 0.45              |
| 1:f:376:GLU:OE1   | 1:f:376:GLU:HA    | 2.17                     | 0.45              |
| 6:Y:51:PRO:HB2    | 6:Y:58:CYS:HA     | 1.99                     | 0.45              |
| 6:Y:508:LEU:HD11  | 6:Y:725:MET:HG2   | 1.99                     | 0.45              |
| 1:a:56:GLU:HA     | 1:a:93:THR:HG22   | 1.99                     | 0.45              |
| 1:c:124:PRO:O     | 1:c:127:ALA:HB3   | 2.17                     | 0.45              |
| 1:e:247:ILE:O     | 1:e:251:LYS:HG3   | 2.17                     | 0.45              |
| 1:f:262:ILE:HB    | 1:f:315:ILE:HG22  | 1.99                     | 0.45              |
| 5:X:93:SER:HA     | 5:X:128:PRO:HA    | 1.98                     | 0.45              |
| 5:X:468:LEU:HA    | 5:X:471:VAL:HG22  | 1.98                     | 0.45              |
| 6:Y:597:GLY:H     | 6:Y:600:ALA:HB3   | 1.81                     | 0.45              |
| 6:Y:1175:LEU:HD22 | 6:Y:1190:ILE:HD11 | 1.98                     | 0.45              |
| 1:c:376:GLU:OE1   | 1:c:376:GLU:HA    | 2.17                     | 0.45              |
| 1:d:247:ILE:O     | 1:d:251:LYS:HG3   | 2.17                     | 0.45              |
| 2:A:389:MET:HA    | 2:A:392:LEU:HB2   | 1.99                     | 0.45              |
| 1:c:265:ASP:HA    | 1:c:266:SER:HA    | 1.49                     | 0.44              |
| 1:d:265:ASP:HA    | 1:d:266:SER:HA    | 1.49                     | 0.44              |
| 1:f:27:ALA:HB3    | 1:f:28:ARG:HH12   | 1.82                     | 0.44              |
| 1:f:91:LEU:HD13   | 1:f:97:ILE:HD11   | 1.99                     | 0.44              |
| 1:f:124:PRO:O     | 1:f:127:ALA:HB3   | 2.17                     | 0.44              |
| 3:U:53:GLY:HA3    | 3:U:177:TYR:HB2   | 1.99                     | 0.44              |
| 6:Y:73:GLY:O      | 6:Y:76:LYS:NZ     | 2.38                     | 0.44              |
| 1:a:376:GLU:OE1   | 1:a:376:GLU:HA    | 2.17                     | 0.44              |
| 1:b:27:ALA:HB3    | 1:b:28:ARG:HH12   | 1.82                     | 0.44              |
| 1:c:292:ASN:OD1   | 1:c:292:ASN:N     | 2.42                     | 0.44              |
| 1:f:247:ILE:O     | 1:f:251:LYS:HG3   | 2.17                     | 0.44              |
| 2:A:27:LEU:HD12   | 2:A:51:ARG:HH12   | 1.83                     | 0.44              |
| 5:X:1023:HIS:O    | 5:X:1026:GLU:HG2  | 2.17                     | 0.44              |
| 5:X:1323:PHE:CD1  | 5:X:1326:LEU:HD21 | 2.52                     | 0.44              |
| 1:a:204:LEU:HD12  | 1:a:261:ILE:HB    | 2.00                     | 0.44              |
| 1:b:166:SER:HB2   | 1:b:341:MET:HE1   | 1.98                     | 0.44              |
| 1:b:204:LEU:HD12  | 1:b:261:ILE:HB    | 2.00                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:d:73:LEU:HD22  | 1:d:238:ARG:NH2   | 2.32                     | 0.44              |
| 1:e:91:LEU:HD13  | 1:e:97:ILE:HD11   | 1.99                     | 0.44              |
| 3:U:48:LEU:HB2   | 5:X:1083:GLU:HB3  | 2.00                     | 0.44              |
| 3:V:188:GLU:HG3  | 3:V:200:LYS:HB3   | 1.98                     | 0.44              |
| 5:X:192:ASP:OD1  | 5:X:192:ASP:N     | 2.48                     | 0.44              |
| 5:X:406:ASN:OD1  | 5:X:411:ARG:NH2   | 2.47                     | 0.44              |
| 5:X:1190:ALA:HB1 | 5:X:1194:GLU:HG2  | 1.99                     | 0.44              |
| 5:X:1326:LEU:HA  | 5:X:1329:GLU:CD   | 2.42                     | 0.44              |
| 1:a:73:LEU:HD22  | 1:a:238:ARG:NH2   | 2.32                     | 0.44              |
| 1:d:31:LYS:HB2   | 1:d:31:LYS:HE2    | 1.45                     | 0.44              |
| 1:d:234:GLU:HB2  | 1:d:238:ARG:HB2   | 1.98                     | 0.44              |
| 1:e:73:LEU:HD22  | 1:e:238:ARG:NH2   | 2.32                     | 0.44              |
| 5:X:44:GLU:HG2   | 5:X:46:GLN:HG2    | 1.99                     | 0.44              |
| 5:X:685:MET:SD   | 5:X:1073:LYS:HE3  | 2.58                     | 0.44              |
| 1:a:247:ILE:O    | 1:a:251:LYS:HG3   | 2.17                     | 0.44              |
| 1:a:309:GLU:H    | 1:a:309:GLU:HG2   | 1.52                     | 0.44              |
| 1:b:376:GLU:HA   | 1:b:376:GLU:OE1   | 2.17                     | 0.44              |
| 1:c:27:ALA:HB3   | 1:c:28:ARG:HH12   | 1.82                     | 0.44              |
| 1:c:262:ILE:HB   | 1:c:315:ILE:HG22  | 1.99                     | 0.44              |
| 1:e:40:LYS:HE2   | 1:e:40:LYS:HB3    | 1.86                     | 0.44              |
| 1:f:166:SER:HB2  | 1:f:341:MET:HE1   | 1.98                     | 0.44              |
| 2:A:40:GLU:OE2   | 2:A:41:GLN:NE2    | 2.50                     | 0.44              |
| 3:V:111:THR:OG1  | 3:V:112:ALA:N     | 2.51                     | 0.44              |
| 3:V:155:ALA:HB1  | 3:V:172:LEU:HD21  | 1.99                     | 0.44              |
| 1:a:179:PRO:O    | 1:a:184:LYS:NZ    | 2.45                     | 0.44              |
| 1:b:73:LEU:HD22  | 1:b:238:ARG:NH2   | 2.32                     | 0.44              |
| 1:c:179:PRO:O    | 1:c:184:LYS:NZ    | 2.45                     | 0.44              |
| 1:f:134:GLU:OE1  | 1:f:134:GLU:N     | 2.47                     | 0.44              |
| 5:X:1088:ASP:OD1 | 5:X:1092:THR:N    | 2.50                     | 0.44              |
| 5:X:1172:LEU:O   | 5:X:1176:LEU:HD23 | 2.18                     | 0.44              |
| 6:Y:54:ASP:OD1   | 6:Y:54:ASP:N      | 2.51                     | 0.44              |
| 1:d:376:GLU:HA   | 1:d:376:GLU:OE1   | 2.17                     | 0.44              |
| 1:e:376:GLU:OE1  | 1:e:376:GLU:HA    | 2.17                     | 0.44              |
| 5:X:55:SER:OG    | 5:X:465:ARG:NH1   | 2.51                     | 0.44              |
| 5:X:155:VAL:HG12 | 5:X:176:ILE:HG12  | 2.00                     | 0.44              |
| 5:X:488:MET:O    | 5:X:490:GLN:N     | 2.43                     | 0.44              |
| 5:X:854:ILE:HB   | 5:X:857:VAL:HG11  | 1.99                     | 0.44              |
| 5:X:1180:MET:HE3 | 5:X:1181:PRO:HD2  | 2.00                     | 0.44              |
| 6:Y:641:ILE:HD11 | 6:Y:764:ARG:HG3   | 1.99                     | 0.44              |
| 1:a:91:LEU:HD13  | 1:a:97:ILE:HD11   | 1.99                     | 0.44              |
| 1:a:95:ASP:HB3   | 1:a:97:ILE:HG12   | 1.99                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:a:262:ILE:HB   | 1:a:315:ILE:HG22  | 1.99                     | 0.44              |
| 1:b:265:ASP:HA   | 1:b:266:SER:HA    | 1.49                     | 0.44              |
| 1:c:91:LEU:HD13  | 1:c:97:ILE:HD11   | 1.99                     | 0.44              |
| 1:c:234:GLU:HB2  | 1:c:238:ARG:HB2   | 1.98                     | 0.44              |
| 1:c:247:ILE:O    | 1:c:251:LYS:HG3   | 2.17                     | 0.44              |
| 1:e:27:ALA:HB3   | 1:e:28:ARG:HH12   | 1.82                     | 0.44              |
| 1:e:140:HIS:CE1  | 1:f:214:GLU:HG3   | 2.53                     | 0.44              |
| 1:e:262:ILE:HB   | 1:e:315:ILE:HG22  | 1.99                     | 0.44              |
| 1:e:309:GLU:H    | 1:e:309:GLU:HG2   | 1.52                     | 0.44              |
| 2:A:409:ARG:HA   | 2:A:412:ASN:ND2   | 2.33                     | 0.44              |
| 3:U:62:ASP:OD1   | 3:U:62:ASP:N      | 2.50                     | 0.44              |
| 6:Y:180:MET:HE2  | 6:Y:180:MET:HB3   | 1.80                     | 0.44              |
| 6:Y:368:LEU:HB2  | 6:Y:439:PRO:HB3   | 2.00                     | 0.44              |
| 6:Y:805:GLN:OE1  | 6:Y:1347:LEU:HB2  | 2.18                     | 0.44              |
| 1:b:56:GLU:HA    | 1:b:93:THR:HG22   | 1.99                     | 0.44              |
| 1:d:27:ALA:HB3   | 1:d:28:ARG:HH12   | 1.82                     | 0.44              |
| 1:d:173:ARG:HG3  | 1:d:315:ILE:HD11  | 2.00                     | 0.44              |
| 1:f:173:ARG:HG3  | 1:f:315:ILE:HD11  | 2.00                     | 0.44              |
| 1:f:266:SER:OG   | 1:f:267:ILE:N     | 2.49                     | 0.44              |
| 2:A:255:ARG:HD2  | 2:A:255:ARG:HA    | 1.78                     | 0.44              |
| 2:A:428:ASN:HD21 | 2:A:450:ALA:HB2   | 1.82                     | 0.44              |
| 3:V:15:ASP:H     | 3:V:27:THR:HG22   | 1.83                     | 0.44              |
| 5:X:811:ASN:ND2  | 5:X:1098:LEU:O    | 2.45                     | 0.44              |
| 5:X:979:LEU:HD13 | 5:X:1000:LEU:HD12 | 1.99                     | 0.44              |
| 1:c:73:LEU:HD22  | 1:c:238:ARG:NH2   | 2.32                     | 0.43              |
| 1:c:171:GLY:N    | 1:c:314:THR:HG1   | 2.16                     | 0.43              |
| 1:c:204:LEU:HD12 | 1:c:261:ILE:HB    | 2.00                     | 0.43              |
| 1:f:73:LEU:HD22  | 1:f:238:ARG:NH2   | 2.32                     | 0.43              |
| 1:f:172:GLN:NE2  | 1:f:340:ASN:OD1   | 2.47                     | 0.43              |
| 1:f:292:ASN:OD1  | 1:f:292:ASN:N     | 2.42                     | 0.43              |
| 2:A:186:VAL:C    | 2:A:187:ARG:HD2   | 2.43                     | 0.43              |
| 2:A:221:ILE:HG23 | 2:A:240:THR:HG22  | 2.00                     | 0.43              |
| 5:X:174:ALA:HB2  | 5:X:432:LEU:HD13  | 1.99                     | 0.43              |
| 5:X:229:ILE:O    | 5:X:239:MET:HG3   | 2.18                     | 0.43              |
| 5:X:685:MET:SD   | 5:X:1073:LYS:HB3  | 2.58                     | 0.43              |
| 1:b:339:GLY:O    | 1:c:212:ARG:NH2   | 2.51                     | 0.43              |
| 1:c:323:THR:OG1  | 1:c:328:ASP:OD2   | 2.28                     | 0.43              |
| 1:f:240:VAL:HG23 | 1:f:274:TYR:CE1   | 2.53                     | 0.43              |
| 2:A:80:ALA:HB1   | 2:A:86:SER:N      | 2.33                     | 0.43              |
| 3:U:120:ASP:N    | 3:U:120:ASP:OD1   | 2.49                     | 0.43              |
| 5:X:158:ASP:OD1  | 5:X:159:SER:N     | 2.52                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:Y:338:PHE:HA    | 6:Y:342:LEU:HD12 | 2.00                     | 0.43              |
| 1:b:247:ILE:O     | 1:b:251:LYS:HG3  | 2.17                     | 0.43              |
| 3:U:111:THR:OG1   | 3:U:112:ALA:N    | 2.52                     | 0.43              |
| 3:U:207:THR:OG1   | 3:U:208:ASN:N    | 2.51                     | 0.43              |
| 3:V:29:GLU:HA     | 3:V:30:PRO:HA    | 1.75                     | 0.43              |
| 5:X:995:ASP:OD1   | 5:X:996:ARG:NH2  | 2.49                     | 0.43              |
| 6:Y:684:ASP:OD1   | 6:Y:684:ASP:N    | 2.47                     | 0.43              |
| 6:Y:789:LYS:NZ    | 6:Y:927:GLY:O    | 2.46                     | 0.43              |
| 6:Y:945:ALA:HB1   | 6:Y:1023:HIS:HB3 | 2.00                     | 0.43              |
| 1:a:382:ILE:HG13  | 1:a:383:LEU:N    | 2.31                     | 0.43              |
| 1:b:184:LYS:O     | 1:b:188:LEU:HG   | 2.19                     | 0.43              |
| 1:c:95:ASP:HB3    | 1:c:97:ILE:HG12  | 1.99                     | 0.43              |
| 1:d:240:VAL:HG23  | 1:d:274:TYR:CE1  | 2.54                     | 0.43              |
| 1:e:234:GLU:HB2   | 1:e:238:ARG:HB2  | 1.98                     | 0.43              |
| 1:f:7:LYS:HD3     | 1:f:69:ASP:HB3   | 2.01                     | 0.43              |
| 1:f:95:ASP:HB3    | 1:f:97:ILE:HG12  | 1.99                     | 0.43              |
| 2:A:104:ARG:HA    | 2:A:104:ARG:HD2  | 1.76                     | 0.43              |
| 2:A:476:GLU:H     | 2:A:476:GLU:CD   | 2.26                     | 0.43              |
| 5:X:423:ASP:OD1   | 5:X:423:ASP:N    | 2.52                     | 0.43              |
| 5:X:638:SER:OG    | 5:X:639:LYS:N    | 2.50                     | 0.43              |
| 5:X:1256:GLN:OE1  | 6:Y:99:ARG:NH2   | 2.51                     | 0.43              |
| 5:X:1339:LEU:HD23 | 6:Y:20:ILE:HG23  | 1.99                     | 0.43              |
| 6:Y:973:LEU:HB3   | 6:Y:1003:LEU:HB3 | 2.00                     | 0.43              |
| 1:a:171:GLY:N     | 1:a:314:THR:OG1  | 2.38                     | 0.43              |
| 1:a:184:LYS:O     | 1:a:188:LEU:HG   | 2.19                     | 0.43              |
| 1:b:95:ASP:HB3    | 1:b:97:ILE:HG12  | 1.99                     | 0.43              |
| 1:c:75:GLY:N      | 1:c:78:ASP:OD2   | 2.47                     | 0.43              |
| 1:c:240:VAL:HG23  | 1:c:274:TYR:CE1  | 2.54                     | 0.43              |
| 1:c:283:LYS:NZ    | 1:d:276:THR:O    | 2.49                     | 0.43              |
| 1:d:292:ASN:OD1   | 1:d:292:ASN:N    | 2.42                     | 0.43              |
| 1:e:382:ILE:HG13  | 1:e:383:LEU:N    | 2.31                     | 0.43              |
| 1:f:60:ASP:OD1    | 1:f:61:GLY:N     | 2.48                     | 0.43              |
| 3:U:45:ARG:HD3    | 3:V:38:THR:HB    | 1.99                     | 0.43              |
| 4:W:38:LEU:HD23   | 4:W:58:LEU:HD23  | 2.00                     | 0.43              |
| 5:X:202:ARG:HH21  | 5:X:369:MET:HA   | 1.83                     | 0.43              |
| 5:X:946:LEU:O     | 5:X:949:GLU:HG3  | 2.18                     | 0.43              |
| 5:X:1281:TYR:CD2  | 6:Y:484:MET:HE3  | 2.54                     | 0.43              |
| 6:Y:93:THR:OG1    | 6:Y:94:GLN:N     | 2.51                     | 0.43              |
| 6:Y:1134:ILE:HD12 | 6:Y:1134:ILE:H   | 1.83                     | 0.43              |
| 1:a:220:GLN:HA    | 1:a:227:VAL:HG11 | 2.01                     | 0.43              |
| 1:c:15:ILE:HG21   | 1:c:27:ALA:HB2   | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:d:15:ILE:HG21   | 1:d:27:ALA:HB2    | 2.01                     | 0.43              |
| 5:X:11:ILE:HG22   | 5:X:1172:LEU:HD11 | 2.01                     | 0.43              |
| 5:X:543:ALA:HB3   | 5:X:548:ARG:HH21  | 1.83                     | 0.43              |
| 6:Y:640:GLY:N     | 6:Y:643:ASP:OD2   | 2.51                     | 0.43              |
| 1:b:172:GLN:NE2   | 1:b:340:ASN:OD1   | 2.47                     | 0.43              |
| 1:c:173:ARG:HG3   | 1:c:315:ILE:HD11  | 2.00                     | 0.43              |
| 1:e:31:LYS:HB2    | 1:e:31:LYS:HE2    | 1.45                     | 0.43              |
| 1:e:204:LEU:HD12  | 1:e:261:ILE:HB    | 2.00                     | 0.43              |
| 2:A:63:LEU:HB3    | 2:A:73:LYS:HB2    | 1.99                     | 0.43              |
| 3:U:295:LEU:HD23  | 3:U:295:LEU:HA    | 1.79                     | 0.43              |
| 6:Y:1191:PRO:HD2  | 6:Y:1194:ARG:NH2  | 2.33                     | 0.43              |
| 1:b:60:ASP:OD1    | 1:b:61:GLY:N      | 2.48                     | 0.43              |
| 1:d:95:ASP:HB3    | 1:d:97:ILE:HG12   | 1.99                     | 0.43              |
| 1:d:243:ALA:C     | 1:d:300:PHE:HZ    | 2.27                     | 0.43              |
| 1:e:231:THR:HG23  | 1:e:233:ASP:H     | 1.84                     | 0.43              |
| 1:e:292:ASN:OD1   | 1:e:292:ASN:N     | 2.42                     | 0.43              |
| 1:f:184:LYS:O     | 1:f:188:LEU:HG    | 2.19                     | 0.43              |
| 2:A:65:VAL:N      | 2:A:75:ILE:O      | 2.52                     | 0.43              |
| 5:X:303:ASP:OD1   | 5:X:328:SER:OG    | 2.37                     | 0.43              |
| 6:Y:311:ARG:NH2   | 8:L:-2:DC:OP1     | 2.50                     | 0.43              |
| 6:Y:1275:LEU:HB3  | 6:Y:1278:GLU:HG2  | 1.99                     | 0.43              |
| 1:d:90:ASN:ND2    | 1:e:28:ARG:HB3    | 2.34                     | 0.43              |
| 1:e:166:SER:HB3   | 1:e:365:THR:OG1   | 2.19                     | 0.43              |
| 1:e:240:VAL:HG23  | 1:e:274:TYR:CE1   | 2.53                     | 0.43              |
| 1:f:204:LEU:HD12  | 1:f:261:ILE:HB    | 2.00                     | 0.43              |
| 2:A:432:ASP:OD1   | 2:A:433:ASP:N     | 2.51                     | 0.43              |
| 3:U:179:PRO:C     | 3:U:207:THR:HG1   | 2.22                     | 0.43              |
| 5:X:180:ARG:NH2   | 5:X:396:ASP:OD2   | 2.50                     | 0.43              |
| 5:X:1151:LEU:HD11 | 5:X:1198:LEU:HD13 | 2.01                     | 0.43              |
| 6:Y:204:GLU:HG3   | 6:Y:217:LEU:HD21  | 1.99                     | 0.43              |
| 6:Y:705:THR:OG1   | 6:Y:718:SER:OG    | 2.31                     | 0.43              |
| 7:K:0:DT:H2"      | 7:K:1:DT:C6       | 2.54                     | 0.43              |
| 1:b:240:VAL:HG23  | 1:b:274:TYR:CE1   | 2.53                     | 0.43              |
| 1:c:237:SER:O     | 1:c:240:VAL:HG12  | 2.19                     | 0.43              |
| 1:d:134:GLU:OE1   | 1:d:134:GLU:N     | 2.47                     | 0.43              |
| 3:V:205:MET:HG3   | 3:V:213:PRO:HB3   | 2.01                     | 0.43              |
| 5:X:63:SER:O      | 5:X:63:SER:OG     | 2.33                     | 0.43              |
| 5:X:1340:GLU:HG3  | 6:Y:1341:ARG:HE   | 1.84                     | 0.43              |
| 6:Y:255:LEU:HB3   | 6:Y:260:PHE:HA    | 2.01                     | 0.43              |
| 1:a:243:ALA:C     | 1:a:300:PHE:HZ    | 2.27                     | 0.42              |
| 1:a:383:LEU:HD23  | 1:a:413:PHE:CE1   | 2.54                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:c:134:GLU:OE1   | 1:c:134:GLU:N    | 2.47                     | 0.42              |
| 1:c:184:LYS:O     | 1:c:188:LEU:HG   | 2.19                     | 0.42              |
| 1:c:231:THR:HG23  | 1:c:233:ASP:H    | 1.84                     | 0.42              |
| 1:c:383:LEU:HD23  | 1:c:413:PHE:CE1  | 2.54                     | 0.42              |
| 1:d:231:THR:HG23  | 1:d:233:ASP:H    | 1.84                     | 0.42              |
| 1:e:237:SER:O     | 1:e:240:VAL:HG12 | 2.19                     | 0.42              |
| 1:f:220:GLN:HA    | 1:f:227:VAL:HG11 | 2.01                     | 0.42              |
| 1:a:75:GLY:N      | 1:a:78:ASP:OD2   | 2.47                     | 0.42              |
| 1:a:237:SER:O     | 1:a:240:VAL:HG12 | 2.19                     | 0.42              |
| 1:b:15:ILE:HG21   | 1:b:27:ALA:HB2   | 2.01                     | 0.42              |
| 1:b:164:LEU:CD1   | 1:b:403:LEU:HD21 | 2.49                     | 0.42              |
| 1:b:230:SER:OG    | 1:b:239:HIS:ND1  | 2.53                     | 0.42              |
| 1:b:237:SER:O     | 1:b:240:VAL:HG12 | 2.19                     | 0.42              |
| 1:c:7:LYS:HD3     | 1:c:69:ASP:HB3   | 2.01                     | 0.42              |
| 1:e:173:ARG:HG3   | 1:e:315:ILE:HD11 | 2.00                     | 0.42              |
| 1:f:15:ILE:HG21   | 1:f:27:ALA:HB2   | 2.01                     | 0.42              |
| 1:f:171:GLY:N     | 1:f:314:THR:HG1  | 2.15                     | 0.42              |
| 5:X:1223:ARG:HH21 | 6:Y:515:ARG:HH12 | 1.67                     | 0.42              |
| 6:Y:107:LEU:HD11  | 6:Y:299:LEU:HD11 | 2.01                     | 0.42              |
| 1:a:164:LEU:CD1   | 1:a:403:LEU:HD21 | 2.49                     | 0.42              |
| 1:a:166:SER:HB3   | 1:a:365:THR:OG1  | 2.19                     | 0.42              |
| 1:d:7:LYS:HD3     | 1:d:69:ASP:HB3   | 2.01                     | 0.42              |
| 1:d:166:SER:HB3   | 1:d:365:THR:OG1  | 2.19                     | 0.42              |
| 1:d:204:LEU:HD12  | 1:d:261:ILE:HB   | 2.00                     | 0.42              |
| 5:X:452:ARG:NH2   | 5:X:458:GLU:OE2  | 2.48                     | 0.42              |
| 5:X:1040:ASP:OD1  | 5:X:1040:ASP:N   | 2.48                     | 0.42              |
| 6:Y:113:HIS:CE1   | 6:Y:307:LEU:HD13 | 2.54                     | 0.42              |
| 6:Y:811:GLU:O     | 6:Y:896:ALA:N    | 2.40                     | 0.42              |
| 1:a:173:ARG:HG3   | 1:a:315:ILE:HD11 | 2.00                     | 0.42              |
| 1:a:240:VAL:HG23  | 1:a:274:TYR:CE1  | 2.54                     | 0.42              |
| 1:b:75:GLY:N      | 1:b:78:ASP:OD2   | 2.47                     | 0.42              |
| 1:e:95:ASP:HB3    | 1:e:97:ILE:HG12  | 2.00                     | 0.42              |
| 1:e:164:LEU:CD1   | 1:e:403:LEU:HD21 | 2.49                     | 0.42              |
| 1:e:220:GLN:HA    | 1:e:227:VAL:HG11 | 2.01                     | 0.42              |
| 1:f:383:LEU:HD23  | 1:f:413:PHE:CE1  | 2.54                     | 0.42              |
| 3:V:46:ILE:HD11   | 3:V:224:LEU:HD13 | 2.01                     | 0.42              |
| 5:X:957:LYS:HB2   | 5:X:957:LYS:HE3  | 1.84                     | 0.42              |
| 6:Y:789:LYS:HB3   | 6:Y:789:LYS:HE3  | 1.72                     | 0.42              |
| 6:Y:1037:PHE:HA   | 6:Y:1040:MET:HE2 | 2.01                     | 0.42              |
| 6:Y:1140:ARG:NH2  | 6:Y:1236:GLU:OE2 | 2.52                     | 0.42              |
| 1:a:292:ASN:OD1   | 1:a:292:ASN:N    | 2.42                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:b:243:ALA:C     | 1:b:300:PHE:HZ    | 2.27                     | 0.42              |
| 1:f:164:LEU:CD1   | 1:f:403:LEU:HD21  | 2.49                     | 0.42              |
| 2:A:127:VAL:HG11  | 2:A:188:PRO:O     | 2.20                     | 0.42              |
| 5:X:251:ALA:HB3   | 5:X:267:ARG:H     | 1.84                     | 0.42              |
| 5:X:1246:ARG:NH1  | 5:X:1266:GLY:HA2  | 2.30                     | 0.42              |
| 6:Y:575:GLY:O     | 6:Y:578:ILE:HG12  | 2.20                     | 0.42              |
| 6:Y:883:ARG:NH1   | 6:Y:898:CYS:SG    | 2.86                     | 0.42              |
| 1:a:123:LYS:HG3   | 1:a:125:GLU:H     | 1.85                     | 0.42              |
| 1:b:177:VAL:HG12  | 1:b:321:ILE:HD13  | 2.02                     | 0.42              |
| 1:c:164:LEU:CD1   | 1:c:403:LEU:HD21  | 2.49                     | 0.42              |
| 1:c:220:GLN:HA    | 1:c:227:VAL:HG11  | 2.01                     | 0.42              |
| 1:d:185:THR:HA    | 1:d:188:LEU:CD1   | 2.50                     | 0.42              |
| 1:e:7:LYS:HD3     | 1:e:69:ASP:HB3    | 2.00                     | 0.42              |
| 3:V:159:ILE:HB    | 3:V:172:LEU:HD13  | 2.02                     | 0.42              |
| 5:X:300:ASP:HB3   | 5:X:309:LEU:HD11  | 2.02                     | 0.42              |
| 5:X:1105:SER:HB3  | 6:Y:731:ARG:HG3   | 2.00                     | 0.42              |
| 5:X:1115:THR:HG22 | 5:X:1228:GLY:HA3  | 2.01                     | 0.42              |
| 5:X:1225:VAL:HG23 | 6:Y:638:SER:OG    | 2.19                     | 0.42              |
| 5:X:1246:ARG:CZ   | 5:X:1258:PRO:HB3  | 2.50                     | 0.42              |
| 5:X:1277:ALA:HA   | 6:Y:921:GLN:HE22  | 1.84                     | 0.42              |
| 5:X:1287:LEU:HD13 | 6:Y:1357:ILE:HD11 | 2.02                     | 0.42              |
| 6:Y:161:THR:H     | 6:Y:164:GLN:HB2   | 1.84                     | 0.42              |
| 1:a:7:LYS:HD3     | 1:a:69:ASP:HB3    | 2.01                     | 0.42              |
| 1:a:231:THR:HG23  | 1:a:233:ASP:H     | 1.84                     | 0.42              |
| 1:b:231:THR:HG23  | 1:b:233:ASP:H     | 1.84                     | 0.42              |
| 1:c:130:LYS:HG2   | 1:d:28:ARG:HH21   | 1.84                     | 0.42              |
| 1:d:220:GLN:HA    | 1:d:227:VAL:HG11  | 2.01                     | 0.42              |
| 1:d:243:ALA:O     | 1:d:300:PHE:HZ    | 2.03                     | 0.42              |
| 1:e:123:LYS:HG3   | 1:e:125:GLU:H     | 1.85                     | 0.42              |
| 1:e:184:LYS:O     | 1:e:188:LEU:HG    | 2.19                     | 0.42              |
| 1:f:166:SER:HB3   | 1:f:365:THR:OG1   | 2.19                     | 0.42              |
| 2:A:62:TRP:HD1    | 2:A:91:ASP:O      | 2.03                     | 0.42              |
| 2:A:78:GLU:O      | 2:A:80:ALA:N      | 2.51                     | 0.42              |
| 3:U:232:VAL:HG23  | 3:V:221:ALA:HB3   | 2.01                     | 0.42              |
| 1:c:177:VAL:HG12  | 1:c:321:ILE:HD13  | 2.02                     | 0.42              |
| 1:e:15:ILE:HG21   | 1:e:27:ALA:HB2    | 2.01                     | 0.42              |
| 1:e:185:THR:HA    | 1:e:188:LEU:CD1   | 2.50                     | 0.42              |
| 1:e:243:ALA:O     | 1:e:300:PHE:HZ    | 2.03                     | 0.42              |
| 1:e:383:LEU:HD23  | 1:e:413:PHE:CE1   | 2.54                     | 0.42              |
| 2:A:9:VAL:HG21    | 2:A:51:ARG:HD3    | 2.02                     | 0.42              |
| 2:A:283:PHE:CZ    | 2:A:331:LEU:HB3   | 2.54                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:V:70:THR:HG23  | 3:V:70:THR:O      | 2.20                     | 0.42              |
| 6:Y:1292:LEU:HA  | 6:Y:1297:LYS:HZ3  | 1.84                     | 0.42              |
| 1:a:83:PRO:CD    | 8:L:19:DG:H2''    | 2.49                     | 0.42              |
| 1:b:166:SER:HB3  | 1:b:365:THR:OG1   | 2.19                     | 0.42              |
| 1:b:220:GLN:HA   | 1:b:227:VAL:HG11  | 2.01                     | 0.42              |
| 1:d:75:GLY:N     | 1:d:78:ASP:OD2    | 2.47                     | 0.42              |
| 1:d:237:SER:O    | 1:d:240:VAL:HG12  | 2.19                     | 0.42              |
| 5:X:163:LYS:HD2  | 5:X:163:LYS:HA    | 1.88                     | 0.42              |
| 5:X:387:ASN:HA   | 5:X:391:SER:HB3   | 2.02                     | 0.42              |
| 5:X:993:PRO:HB2  | 5:X:997:TRP:NE1   | 2.35                     | 0.42              |
| 5:X:1269:ARG:HB2 | 6:Y:346:ARG:HG2   | 2.02                     | 0.42              |
| 6:Y:270:ARG:HD2  | 7:K:-15:DG:C5'    | 2.48                     | 0.42              |
| 6:Y:825:VAL:HG13 | 6:Y:832:LYS:HB2   | 2.02                     | 0.42              |
| 9:R:82:C:H2'     | 9:R:83:C:C6       | 2.54                     | 0.42              |
| 1:d:164:LEU:CD1  | 1:d:403:LEU:HD21  | 2.49                     | 0.42              |
| 1:d:383:LEU:HD23 | 1:d:413:PHE:CE1   | 2.54                     | 0.42              |
| 1:f:25:ASN:N     | 1:f:25:ASN:OD1    | 2.53                     | 0.42              |
| 1:f:243:ALA:O    | 1:f:300:PHE:HZ    | 2.03                     | 0.42              |
| 2:A:63:LEU:HB3   | 2:A:73:LYS:O      | 2.20                     | 0.42              |
| 2:A:283:PHE:HZ   | 2:A:331:LEU:HB3   | 1.84                     | 0.42              |
| 2:A:393:LEU:H    | 2:A:393:LEU:HD23  | 1.85                     | 0.42              |
| 2:A:449:ALA:HA   | 2:A:453:VAL:O     | 2.20                     | 0.42              |
| 3:U:193:GLU:HG2  | 3:U:194:GLN:N     | 2.35                     | 0.42              |
| 5:X:1323:PHE:O   | 5:X:1327:LEU:HD23 | 2.19                     | 0.42              |
| 6:Y:352:ARG:NH1  | 8:L:4:DC:H4'      | 2.35                     | 0.42              |
| 6:Y:644:MET:HE3  | 6:Y:644:MET:HB2   | 1.93                     | 0.42              |
| 6:Y:845:ALA:HB2  | 6:Y:883:ARG:HG2   | 2.01                     | 0.42              |
| 6:Y:857:LEU:HD23 | 6:Y:857:LEU:H     | 1.85                     | 0.42              |
| 6:Y:871:LEU:O    | 6:Y:875:ASN:ND2   | 2.49                     | 0.42              |
| 1:a:83:PRO:HG2   | 8:L:19:DG:H2''    | 2.02                     | 0.41              |
| 1:a:212:ARG:O    | 1:a:216:VAL:HG23  | 2.20                     | 0.41              |
| 1:b:185:THR:HA   | 1:b:188:LEU:CD1   | 2.50                     | 0.41              |
| 1:b:383:LEU:HD23 | 1:b:413:PHE:CE1   | 2.54                     | 0.41              |
| 1:c:25:ASN:OD1   | 1:c:25:ASN:N      | 2.53                     | 0.41              |
| 1:c:166:SER:HB3  | 1:c:365:THR:OG1   | 2.19                     | 0.41              |
| 1:c:212:ARG:O    | 1:c:216:VAL:HG23  | 2.20                     | 0.41              |
| 1:c:243:ALA:O    | 1:c:300:PHE:HZ    | 2.03                     | 0.41              |
| 1:c:243:ALA:C    | 1:c:300:PHE:HZ    | 2.27                     | 0.41              |
| 1:d:184:LYS:O    | 1:d:188:LEU:HG    | 2.19                     | 0.41              |
| 1:d:212:ARG:O    | 1:d:216:VAL:HG23  | 2.20                     | 0.41              |
| 2:A:9:VAL:HG23   | 2:A:23:ILE:HG21   | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:14:ASN:HB3    | 2:A:17:ALA:HB3    | 2.02                     | 0.41              |
| 2:A:123:ARG:HA    | 2:A:126:VAL:HG12  | 2.02                     | 0.41              |
| 2:A:127:VAL:HA    | 2:A:130:PHE:HB3   | 2.02                     | 0.41              |
| 2:A:203:GLU:HA    | 2:A:206:ILE:CG1   | 2.49                     | 0.41              |
| 5:X:434:ASP:HB3   | 5:X:439:LYS:HG3   | 2.02                     | 0.41              |
| 5:X:675:ASP:OD1   | 5:X:676:ALA:N     | 2.52                     | 0.41              |
| 5:X:781:ASP:OD1   | 5:X:782:VAL:N     | 2.54                     | 0.41              |
| 5:X:1119:MET:HE1  | 5:X:1208:GLY:HA2  | 2.02                     | 0.41              |
| 6:Y:1132:LYS:HE2  | 6:Y:1152:GLU:H    | 1.85                     | 0.41              |
| 6:Y:1343:GLU:C    | 6:Y:1344:LEU:HD23 | 2.45                     | 0.41              |
| 1:b:173:ARG:HG3   | 1:b:315:ILE:HD11  | 2.00                     | 0.41              |
| 1:c:60:ASP:OD1    | 1:c:61:GLY:N      | 2.48                     | 0.41              |
| 1:c:123:LYS:HG3   | 1:c:125:GLU:H     | 1.85                     | 0.41              |
| 1:c:172:GLN:NE2   | 1:c:340:ASN:OD1   | 2.47                     | 0.41              |
| 1:e:243:ALA:C     | 1:e:300:PHE:HZ    | 2.27                     | 0.41              |
| 2:A:112:GLN:HA    | 2:A:115:VAL:HG12  | 2.01                     | 0.41              |
| 3:U:163:GLU:HA    | 3:U:166:ARG:HG2   | 2.02                     | 0.41              |
| 3:V:229:GLU:HA    | 3:V:232:VAL:HG22  | 2.02                     | 0.41              |
| 5:X:684:ASN:ND2   | 5:X:687:ARG:HH22  | 2.16                     | 0.41              |
| 5:X:972:PHE:O     | 5:X:975:ILE:HG22  | 2.21                     | 0.41              |
| 5:X:1293:VAL:HG21 | 5:X:1315:MET:SD   | 2.59                     | 0.41              |
| 6:Y:740:LEU:HA    | 6:Y:763:PHE:HD2   | 1.84                     | 0.41              |
| 6:Y:812:ASP:HA    | 6:Y:896:ALA:HB3   | 2.02                     | 0.41              |
| 6:Y:1029:THR:HG21 | 6:Y:1115:ILE:HD12 | 2.01                     | 0.41              |
| 6:Y:1268:ASN:H    | 6:Y:1301:THR:HG1  | 1.63                     | 0.41              |
| 1:a:265:ASP:HA    | 1:a:266:SER:HA    | 1.49                     | 0.41              |
| 1:b:123:LYS:HG3   | 1:b:125:GLU:H     | 1.85                     | 0.41              |
| 1:b:243:ALA:O     | 1:b:300:PHE:HZ    | 2.03                     | 0.41              |
| 1:d:25:ASN:OD1    | 1:d:25:ASN:N      | 2.53                     | 0.41              |
| 1:f:54:VAL:HA     | 1:f:95:ASP:O      | 2.20                     | 0.41              |
| 1:f:123:LYS:HG3   | 1:f:125:GLU:H     | 1.85                     | 0.41              |
| 1:f:171:GLY:N     | 1:f:314:THR:OG1   | 2.38                     | 0.41              |
| 2:A:247:PRO:HG2   | 2:A:275:LEU:HD22  | 2.02                     | 0.41              |
| 6:Y:113:HIS:HB3   | 6:Y:116:PHE:CD2   | 2.55                     | 0.41              |
| 6:Y:537:TYR:OH    | 6:Y:634:ARG:NH2   | 2.52                     | 0.41              |
| 6:Y:1156:LEU:CD2  | 6:Y:1209:VAL:HA   | 2.51                     | 0.41              |
| 1:c:295:HIS:CE1   | 1:c:299:ARG:HH21  | 2.39                     | 0.41              |
| 1:f:243:ALA:C     | 1:f:300:PHE:HZ    | 2.27                     | 0.41              |
| 2:A:33:THR:O      | 2:A:37:LYS:NZ     | 2.48                     | 0.41              |
| 5:X:125:GLY:H     | 5:X:495:ALA:HB1   | 1.84                     | 0.41              |
| 5:X:463:GLN:HG3   | 5:X:505:PHE:CG    | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:X:619:ALA:HB3  | 6:Y:769:VAL:HG21 | 2.02                     | 0.41              |
| 5:X:1111:GLN:O   | 5:X:1114:GLU:HB3 | 2.20                     | 0.41              |
| 5:X:1232:MET:HE2 | 5:X:1232:MET:HB3 | 1.99                     | 0.41              |
| 6:Y:43:THR:OG1   | 6:Y:44:ILE:N     | 2.53                     | 0.41              |
| 7:K:5:DA:H2"     | 7:K:6:DG:H8      | 1.85                     | 0.41              |
| 1:a:109:ARG:NH1  | 6:Y:87:LYS:HB3   | 2.35                     | 0.41              |
| 1:a:185:THR:HA   | 1:a:188:LEU:CD1  | 2.50                     | 0.41              |
| 1:b:7:LYS:HD3    | 1:b:69:ASP:HB3   | 2.01                     | 0.41              |
| 1:b:160:ARG:NH1  | 1:b:406:THR:HG23 | 2.30                     | 0.41              |
| 1:b:212:ARG:O    | 1:b:216:VAL:HG23 | 2.20                     | 0.41              |
| 1:d:54:VAL:HA    | 1:d:95:ASP:O     | 2.20                     | 0.41              |
| 1:d:295:HIS:CE1  | 1:d:299:ARG:HH21 | 2.39                     | 0.41              |
| 1:f:29:MET:HB2   | 1:f:33:ASP:HB2   | 2.03                     | 0.41              |
| 1:f:237:SER:O    | 1:f:240:VAL:HG12 | 2.19                     | 0.41              |
| 2:A:9:VAL:O      | 2:A:12:VAL:HG22  | 2.21                     | 0.41              |
| 3:U:91:ARG:HB2   | 3:U:210:THR:HG23 | 2.02                     | 0.41              |
| 5:X:359:ARG:HG2  | 5:X:363:LEU:HD13 | 2.02                     | 0.41              |
| 5:X:448:LEU:HD23 | 5:X:557:ARG:HD2  | 2.02                     | 0.41              |
| 5:X:670:PHE:HB3  | 5:X:673:HIS:HD2  | 1.86                     | 0.41              |
| 5:X:941:LYS:NZ   | 5:X:1037:THR:O   | 2.37                     | 0.41              |
| 7:K:-15:DG:H2"   | 7:K:-14:DC:C6    | 2.55                     | 0.41              |
| 1:a:15:ILE:HG21  | 1:a:27:ALA:HB2   | 2.01                     | 0.41              |
| 1:a:243:ALA:O    | 1:a:300:PHE:HZ   | 2.03                     | 0.41              |
| 1:d:244:GLU:OE1  | 1:d:245:MET:HE2  | 2.21                     | 0.41              |
| 1:e:29:MET:HB2   | 1:e:33:ASP:HB2   | 2.03                     | 0.41              |
| 1:e:54:VAL:HA    | 1:e:95:ASP:O     | 2.20                     | 0.41              |
| 1:f:185:THR:HA   | 1:f:188:LEU:CD1  | 2.50                     | 0.41              |
| 1:f:212:ARG:O    | 1:f:216:VAL:HG23 | 2.20                     | 0.41              |
| 1:f:230:SER:OG   | 1:f:239:HIS:ND1  | 2.53                     | 0.41              |
| 2:A:9:VAL:HG11   | 2:A:51:ARG:HD3   | 2.03                     | 0.41              |
| 1:b:171:GLY:N    | 1:b:314:THR:OG1  | 2.38                     | 0.41              |
| 1:b:295:HIS:CE1  | 1:b:299:ARG:HH21 | 2.39                     | 0.41              |
| 1:c:128:ARG:C    | 1:d:28:ARG:NH1   | 2.77                     | 0.41              |
| 1:c:244:GLU:OE1  | 1:c:245:MET:HE2  | 2.21                     | 0.41              |
| 1:d:60:ASP:OD1   | 1:d:61:GLY:N     | 2.48                     | 0.41              |
| 1:e:212:ARG:O    | 1:e:216:VAL:HG23 | 2.20                     | 0.41              |
| 2:A:66:ASP:HA    | 2:A:76:THR:HG22  | 2.03                     | 0.41              |
| 2:A:380:THR:HG21 | 2:A:383:GLU:HB3  | 2.02                     | 0.41              |
| 2:A:411:LYS:O    | 2:A:411:LYS:HD3  | 2.21                     | 0.41              |
| 5:X:618:GLN:HB3  | 5:X:621:SER:HB3  | 2.03                     | 0.41              |
| 5:X:976:ARG:O    | 5:X:980:VAL:HG13 | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:Y:348:ASP:OD1  | 6:Y:348:ASP:N    | 2.54                     | 0.41              |
| 6:Y:412:LEU:HA   | 6:Y:415:VAL:HG22 | 2.03                     | 0.41              |
| 1:a:54:VAL:HA    | 1:a:95:ASP:O     | 2.20                     | 0.41              |
| 1:a:177:VAL:HG12 | 1:a:321:ILE:HD13 | 2.02                     | 0.41              |
| 1:a:230:SER:OG   | 1:a:239:HIS:ND1  | 2.53                     | 0.41              |
| 1:d:123:LYS:HG3  | 1:d:125:GLU:H    | 1.85                     | 0.41              |
| 1:e:177:VAL:HG12 | 1:e:321:ILE:HD13 | 2.02                     | 0.41              |
| 2:A:111:LYS:O    | 2:A:114:ILE:HG22 | 2.21                     | 0.41              |
| 3:U:92:VAL:O     | 3:U:148:ARG:NH2  | 2.54                     | 0.41              |
| 3:V:180:VAL:O    | 6:Y:535:ARG:NH1  | 2.54                     | 0.41              |
| 5:X:214:ASN:H    | 5:X:359:ARG:HE   | 1.66                     | 0.41              |
| 5:X:1072:ASN:ND2 | 5:X:1111:GLN:OE1 | 2.54                     | 0.41              |
| 6:Y:450:HIS:HB3  | 6:Y:453:VAL:HG12 | 2.01                     | 0.41              |
| 1:b:25:ASN:OD1   | 1:b:25:ASN:N     | 2.53                     | 0.41              |
| 1:b:29:MET:HB2   | 1:b:33:ASP:HB2   | 2.03                     | 0.41              |
| 1:b:125:GLU:O    | 1:b:129:ASN:N    | 2.54                     | 0.41              |
| 1:c:368:GLU:H    | 1:c:368:GLU:HG2  | 1.70                     | 0.41              |
| 1:f:231:THR:HG23 | 1:f:233:ASP:H    | 1.84                     | 0.41              |
| 1:f:368:GLU:H    | 1:f:368:GLU:HG2  | 1.70                     | 0.41              |
| 1:f:383:LEU:HD13 | 1:f:383:LEU:HA   | 1.69                     | 0.41              |
| 2:A:5:ILE:HG22   | 2:A:51:ARG:HH22  | 1.84                     | 0.41              |
| 2:A:76:THR:OG1   | 3:U:286:GLU:OE2  | 2.22                     | 0.41              |
| 2:A:313:ASN:O    | 2:A:317:ALA:N    | 2.52                     | 0.41              |
| 3:U:166:ARG:HA   | 3:U:166:ARG:HD3  | 1.89                     | 0.41              |
| 4:W:15:ASN:HD21  | 4:W:18:ASP:CB    | 2.34                     | 0.41              |
| 5:X:104:ILE:HB   | 5:X:484:LEU:HD22 | 2.03                     | 0.41              |
| 5:X:542:ARG:HB3  | 7:K:0:DT:C2      | 2.55                     | 0.41              |
| 5:X:1072:ASN:OD1 | 5:X:1072:ASN:N   | 2.54                     | 0.41              |
| 5:X:1123:GLY:O   | 5:X:1126:ASP:HB2 | 2.21                     | 0.41              |
| 6:Y:270:ARG:NE   | 7:K:-14:DC:OP1   | 2.54                     | 0.41              |
| 6:Y:334:LYS:HA   | 6:Y:339:ARG:HG2  | 2.02                     | 0.41              |
| 6:Y:907:HIS:ND1  | 6:Y:908:ILE:O    | 2.43                     | 0.41              |
| 1:a:40:LYS:HE2   | 1:a:40:LYS:HB3   | 1.86                     | 0.41              |
| 1:c:333:GLU:OE2  | 1:d:325:SER:HB3  | 2.21                     | 0.41              |
| 1:d:177:VAL:HG12 | 1:d:321:ILE:HD13 | 2.02                     | 0.41              |
| 1:d:283:LYS:NZ   | 1:e:276:THR:O    | 2.42                     | 0.41              |
| 1:e:213:PRO:O    | 1:e:217:THR:HG23 | 2.21                     | 0.41              |
| 1:e:295:HIS:CE1  | 1:e:299:ARG:HH21 | 2.39                     | 0.41              |
| 1:e:302:GLY:HA3  | 1:f:232:PHE:CZ   | 2.55                     | 0.41              |
| 1:f:309:GLU:H    | 1:f:309:GLU:HG2  | 1.52                     | 0.41              |
| 3:U:33:ARG:NH1   | 3:U:197:ASP:OD2  | 2.53                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:U:51:MET:HE3   | 3:U:52:PRO:HD2   | 2.03                     | 0.41              |
| 5:X:211:ARG:HA   | 5:X:215:TYR:HB2  | 2.03                     | 0.41              |
| 5:X:617:ALA:HA   | 5:X:636:CYS:SG   | 2.61                     | 0.41              |
| 6:Y:48:THR:O     | 6:Y:50:LYS:HD2   | 2.21                     | 0.41              |
| 6:Y:587:LEU:HD22 | 6:Y:612:LEU:HD23 | 2.03                     | 0.41              |
| 6:Y:1063:ASP:OD1 | 6:Y:1063:ASP:N   | 2.53                     | 0.41              |
| 1:a:213:PRO:O    | 1:a:217:THR:HG23 | 2.21                     | 0.40              |
| 1:c:29:MET:HB2   | 1:c:33:ASP:HB2   | 2.03                     | 0.40              |
| 1:d:151:ASN:OD1  | 1:d:151:ASN:N    | 2.55                     | 0.40              |
| 1:e:75:GLY:N     | 1:e:78:ASP:OD2   | 2.47                     | 0.40              |
| 1:e:125:GLU:O    | 1:e:129:ASN:N    | 2.54                     | 0.40              |
| 1:e:267:ILE:HG13 | 1:e:318:THR:O    | 2.22                     | 0.40              |
| 1:f:125:GLU:O    | 1:f:129:ASN:N    | 2.54                     | 0.40              |
| 2:A:47:VAL:O     | 2:A:48:GLN:NE2   | 2.53                     | 0.40              |
| 3:U:29:GLU:HA    | 3:U:30:PRO:HA    | 1.85                     | 0.40              |
| 5:X:678:ARG:HD2  | 5:X:1106:ARG:HB3 | 2.03                     | 0.40              |
| 5:X:765:ILE:HG13 | 5:X:787:PRO:HG3  | 2.02                     | 0.40              |
| 5:X:1209:GLN:HG2 | 5:X:1226:THR:HB  | 2.04                     | 0.40              |
| 5:X:1296:ASP:OD2 | 6:Y:345:LYS:NZ   | 2.36                     | 0.40              |
| 1:a:267:ILE:HG13 | 1:a:318:THR:O    | 2.22                     | 0.40              |
| 1:a:302:GLY:HA3  | 1:b:232:PHE:CE1  | 2.56                     | 0.40              |
| 1:e:207:LEU:HB3  | 1:e:263:LEU:O    | 2.22                     | 0.40              |
| 1:f:244:GLU:OE1  | 1:f:245:MET:HE2  | 2.21                     | 0.40              |
| 3:V:142:MET:N    | 3:V:142:MET:SD   | 2.94                     | 0.40              |
| 3:V:236:ASP:OD1  | 3:V:236:ASP:N    | 2.46                     | 0.40              |
| 5:X:1222:GLU:OE2 | 6:Y:512:TYR:OH   | 2.38                     | 0.40              |
| 6:Y:431:ARG:N    | 6:Y:921:GLN:OE1  | 2.54                     | 0.40              |
| 6:Y:1342:ASP:OD1 | 6:Y:1342:ASP:N   | 2.54                     | 0.40              |
| 9:R:77:U:H2'     | 9:R:78:U:H6      | 1.85                     | 0.40              |
| 9:R:92:C:H2'     | 9:R:93:G:H8      | 1.86                     | 0.40              |
| 1:c:54:VAL:HA    | 1:c:95:ASP:O     | 2.21                     | 0.40              |
| 1:c:125:GLU:O    | 1:c:129:ASN:N    | 2.54                     | 0.40              |
| 1:f:267:ILE:HG13 | 1:f:318:THR:O    | 2.22                     | 0.40              |
| 2:A:205:LEU:O    | 2:A:208:LEU:HB2  | 2.21                     | 0.40              |
| 3:U:111:THR:OG1  | 3:U:126:PRO:O    | 2.29                     | 0.40              |
| 5:X:622:ASN:OD1  | 5:X:622:ASN:N    | 2.54                     | 0.40              |
| 6:Y:930:LEU:HD23 | 6:Y:1244:GLN:HG2 | 2.03                     | 0.40              |
| 1:a:25:ASN:OD1   | 1:a:25:ASN:N     | 2.53                     | 0.40              |
| 1:a:60:ASP:OD1   | 1:a:61:GLY:N     | 2.48                     | 0.40              |
| 1:b:292:ASN:OD1  | 1:b:292:ASN:N    | 2.42                     | 0.40              |
| 1:c:160:ARG:NH1  | 1:c:406:THR:HG23 | 2.30                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:e:30:ARG:O     | 1:e:34:ILE:HG13  | 2.22                     | 0.40              |
| 1:e:102:ARG:NH2  | 2:A:83:GLU:HG2   | 2.35                     | 0.40              |
| 2:A:168:LEU:HD11 | 2:A:266:LEU:O    | 2.21                     | 0.40              |
| 2:A:241:ASN:O    | 2:A:243:LYS:NZ   | 2.52                     | 0.40              |
| 3:U:81:ILE:O     | 3:U:85:LEU:HG    | 2.22                     | 0.40              |
| 3:U:104:LYS:HD2  | 3:U:104:LYS:HA   | 1.88                     | 0.40              |
| 3:U:135:ASP:OD1  | 3:U:136:GLU:N    | 2.55                     | 0.40              |
| 3:U:229:GLU:HA   | 3:U:232:VAL:HG12 | 2.03                     | 0.40              |
| 3:V:47:LEU:HD23  | 3:V:47:LEU:HA    | 1.90                     | 0.40              |
| 5:X:193:ASN:ND2  | 5:X:353:VAL:HG11 | 2.36                     | 0.40              |
| 5:X:739:ASP:OD1  | 5:X:740:GLU:N    | 2.51                     | 0.40              |
| 5:X:741:MET:HG2  | 5:X:746:ALA:HB1  | 2.02                     | 0.40              |
| 5:X:930:ASP:HB3  | 5:X:1053:TYR:HD2 | 1.87                     | 0.40              |
| 5:X:1296:ASP:OD2 | 5:X:1322:SER:OG  | 2.26                     | 0.40              |
| 6:Y:1151:LYS:HB2 | 6:Y:1151:LYS:HE2 | 1.88                     | 0.40              |
| 6:Y:1219:ASP:O   | 6:Y:1223:LEU:HG  | 2.21                     | 0.40              |
| 1:b:213:PRO:O    | 1:b:217:THR:HG23 | 2.21                     | 0.40              |
| 1:f:177:VAL:HG12 | 1:f:321:ILE:HD13 | 2.02                     | 0.40              |
| 3:U:184:ALA:HB3  | 3:U:204:GLU:HG2  | 2.04                     | 0.40              |
| 5:X:14:ASP:OD1   | 5:X:15:PHE:N     | 2.54                     | 0.40              |
| 5:X:38:PHE:CD1   | 5:X:48:GLY:HA2   | 2.56                     | 0.40              |
| 5:X:594:VAL:HG13 | 5:X:599:VAL:HG22 | 2.03                     | 0.40              |
| 5:X:657:THR:OG1  | 5:X:1187:PHE:HB2 | 2.21                     | 0.40              |
| 6:Y:703:THR:CG2  | 6:Y:704:GLU:H    | 2.24                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%) | 397 (96%) | 18 (4%) | 0        | <b>100</b> <b>100</b> |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 1   | b     | 415/419 (99%)    | 397 (96%)  | 18 (4%)  | 0        | 100         | 100 |
| 1   | c     | 415/419 (99%)    | 397 (96%)  | 18 (4%)  | 0        | 100         | 100 |
| 1   | d     | 415/419 (99%)    | 397 (96%)  | 18 (4%)  | 0        | 100         | 100 |
| 1   | e     | 415/419 (99%)    | 397 (96%)  | 18 (4%)  | 0        | 100         | 100 |
| 1   | f     | 415/419 (99%)    | 397 (96%)  | 18 (4%)  | 0        | 100         | 100 |
| 2   | A     | 493/497 (99%)    | 453 (92%)  | 40 (8%)  | 0        | 100         | 100 |
| 3   | U     | 320/329 (97%)    | 292 (91%)  | 28 (9%)  | 0        | 100         | 100 |
| 3   | V     | 233/329 (71%)    | 218 (94%)  | 15 (6%)  | 0        | 100         | 100 |
| 4   | W     | 77/91 (85%)      | 72 (94%)   | 5 (6%)   | 0        | 100         | 100 |
| 5   | X     | 1338/1342 (100%) | 1251 (94%) | 87 (6%)  | 0        | 100         | 100 |
| 6   | Y     | 1356/1416 (96%)  | 1302 (96%) | 54 (4%)  | 0        | 100         | 100 |
| All | All   | 6307/6518 (97%)  | 5970 (95%) | 337 (5%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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%)  | 313 (88%)  | 44 (12%) | 4           | 18  |
| 1   | b     | 357/359 (99%)  | 313 (88%)  | 44 (12%) | 4           | 18  |
| 1   | c     | 357/359 (99%)  | 313 (88%)  | 44 (12%) | 4           | 18  |
| 1   | d     | 357/359 (99%)  | 313 (88%)  | 44 (12%) | 4           | 18  |
| 1   | e     | 357/359 (99%)  | 313 (88%)  | 44 (12%) | 4           | 18  |
| 1   | f     | 357/359 (99%)  | 313 (88%)  | 44 (12%) | 4           | 18  |
| 2   | A     | 409/409 (100%) | 409 (100%) | 0        | 100         | 100 |
| 3   | U     | 281/286 (98%)  | 281 (100%) | 0        | 100         | 100 |
| 3   | V     | 203/286 (71%)  | 203 (100%) | 0        | 100         | 100 |
| 4   | W     | 67/75 (89%)    | 67 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 5   | X     | 1155/1157 (100%) | 1155 (100%) | 0        | 100         | 100 |
| 6   | Y     | 1134/1177 (96%)  | 1134 (100%) | 0        | 100         | 100 |
| All | All   | 5391/5544 (97%)  | 5127 (95%)  | 264 (5%) | 24          | 44  |

All (264) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 4   | THR  |
| 1   | a     | 17  | LEU  |
| 1   | a     | 20  | ASN  |
| 1   | a     | 31  | LYS  |
| 1   | a     | 54  | VAL  |
| 1   | a     | 95  | ASP  |
| 1   | a     | 98  | SER  |
| 1   | a     | 114 | LEU  |
| 1   | a     | 154 | THR  |
| 1   | a     | 157 | LEU  |
| 1   | a     | 158 | THR  |
| 1   | a     | 162 | LEU  |
| 1   | a     | 164 | LEU  |
| 1   | a     | 166 | SER  |
| 1   | a     | 186 | MET  |
| 1   | a     | 188 | LEU  |
| 1   | a     | 194 | SER  |
| 1   | a     | 224 | LYS  |
| 1   | a     | 228 | VAL  |
| 1   | a     | 245 | MET  |
| 1   | a     | 265 | ASP  |
| 1   | a     | 281 | SER  |
| 1   | a     | 286 | THR  |
| 1   | a     | 292 | ASN  |
| 1   | a     | 296 | ARG  |
| 1   | a     | 300 | PHE  |
| 1   | a     | 309 | GLU  |
| 1   | a     | 330 | VAL  |
| 1   | a     | 338 | THR  |
| 1   | a     | 346 | SER  |
| 1   | a     | 358 | ILE  |
| 1   | a     | 373 | THR  |
| 1   | a     | 374 | GLN  |
| 1   | a     | 375 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 376 | GLU  |
| 1   | a     | 382 | ILE  |
| 1   | a     | 383 | LEU  |
| 1   | a     | 390 | MET  |
| 1   | a     | 394 | ASP  |
| 1   | a     | 400 | ILE  |
| 1   | a     | 403 | LEU  |
| 1   | a     | 405 | MET  |
| 1   | a     | 409 | ASN  |
| 1   | a     | 411 | ASP  |
| 1   | b     | 4   | THR  |
| 1   | b     | 17  | LEU  |
| 1   | b     | 20  | ASN  |
| 1   | b     | 31  | LYS  |
| 1   | b     | 54  | VAL  |
| 1   | b     | 95  | ASP  |
| 1   | b     | 98  | SER  |
| 1   | b     | 114 | LEU  |
| 1   | b     | 154 | THR  |
| 1   | b     | 157 | LEU  |
| 1   | b     | 158 | THR  |
| 1   | b     | 162 | LEU  |
| 1   | b     | 164 | LEU  |
| 1   | b     | 166 | SER  |
| 1   | b     | 186 | MET  |
| 1   | b     | 188 | LEU  |
| 1   | b     | 194 | SER  |
| 1   | b     | 224 | LYS  |
| 1   | b     | 228 | VAL  |
| 1   | b     | 245 | MET  |
| 1   | b     | 265 | ASP  |
| 1   | b     | 281 | SER  |
| 1   | b     | 286 | THR  |
| 1   | b     | 292 | ASN  |
| 1   | b     | 296 | ARG  |
| 1   | b     | 300 | PHE  |
| 1   | b     | 309 | GLU  |
| 1   | b     | 330 | VAL  |
| 1   | b     | 338 | THR  |
| 1   | b     | 346 | SER  |
| 1   | b     | 358 | ILE  |
| 1   | b     | 373 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | b     | 374 | GLN  |
| 1   | b     | 375 | GLU  |
| 1   | b     | 376 | GLU  |
| 1   | b     | 382 | ILE  |
| 1   | b     | 383 | LEU  |
| 1   | b     | 390 | MET  |
| 1   | b     | 394 | ASP  |
| 1   | b     | 400 | ILE  |
| 1   | b     | 403 | LEU  |
| 1   | b     | 405 | MET  |
| 1   | b     | 409 | ASN  |
| 1   | b     | 411 | ASP  |
| 1   | c     | 4   | THR  |
| 1   | c     | 17  | LEU  |
| 1   | c     | 20  | ASN  |
| 1   | c     | 31  | LYS  |
| 1   | c     | 54  | VAL  |
| 1   | c     | 95  | ASP  |
| 1   | c     | 98  | SER  |
| 1   | c     | 114 | LEU  |
| 1   | c     | 154 | THR  |
| 1   | c     | 157 | LEU  |
| 1   | c     | 158 | THR  |
| 1   | c     | 162 | LEU  |
| 1   | c     | 164 | LEU  |
| 1   | c     | 166 | SER  |
| 1   | c     | 186 | MET  |
| 1   | c     | 188 | LEU  |
| 1   | c     | 194 | SER  |
| 1   | c     | 224 | LYS  |
| 1   | c     | 228 | VAL  |
| 1   | c     | 245 | MET  |
| 1   | c     | 265 | ASP  |
| 1   | c     | 281 | SER  |
| 1   | c     | 286 | THR  |
| 1   | c     | 292 | ASN  |
| 1   | c     | 296 | ARG  |
| 1   | c     | 300 | PHE  |
| 1   | c     | 309 | GLU  |
| 1   | c     | 330 | VAL  |
| 1   | c     | 338 | THR  |
| 1   | c     | 346 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | c     | 358 | ILE  |
| 1   | c     | 373 | THR  |
| 1   | c     | 374 | GLN  |
| 1   | c     | 375 | GLU  |
| 1   | c     | 376 | GLU  |
| 1   | c     | 382 | ILE  |
| 1   | c     | 383 | LEU  |
| 1   | c     | 390 | MET  |
| 1   | c     | 394 | ASP  |
| 1   | c     | 400 | ILE  |
| 1   | c     | 403 | LEU  |
| 1   | c     | 405 | MET  |
| 1   | c     | 409 | ASN  |
| 1   | c     | 411 | ASP  |
| 1   | d     | 4   | THR  |
| 1   | d     | 17  | LEU  |
| 1   | d     | 20  | ASN  |
| 1   | d     | 31  | LYS  |
| 1   | d     | 54  | VAL  |
| 1   | d     | 95  | ASP  |
| 1   | d     | 98  | SER  |
| 1   | d     | 114 | LEU  |
| 1   | d     | 154 | THR  |
| 1   | d     | 157 | LEU  |
| 1   | d     | 158 | THR  |
| 1   | d     | 162 | LEU  |
| 1   | d     | 164 | LEU  |
| 1   | d     | 166 | SER  |
| 1   | d     | 186 | MET  |
| 1   | d     | 188 | LEU  |
| 1   | d     | 194 | SER  |
| 1   | d     | 224 | LYS  |
| 1   | d     | 228 | VAL  |
| 1   | d     | 245 | MET  |
| 1   | d     | 265 | ASP  |
| 1   | d     | 281 | SER  |
| 1   | d     | 286 | THR  |
| 1   | d     | 292 | ASN  |
| 1   | d     | 296 | ARG  |
| 1   | d     | 300 | PHE  |
| 1   | d     | 309 | GLU  |
| 1   | d     | 330 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | d     | 338 | THR  |
| 1   | d     | 346 | SER  |
| 1   | d     | 358 | ILE  |
| 1   | d     | 373 | THR  |
| 1   | d     | 374 | GLN  |
| 1   | d     | 375 | GLU  |
| 1   | d     | 376 | GLU  |
| 1   | d     | 382 | ILE  |
| 1   | d     | 383 | LEU  |
| 1   | d     | 390 | MET  |
| 1   | d     | 394 | ASP  |
| 1   | d     | 400 | ILE  |
| 1   | d     | 403 | LEU  |
| 1   | d     | 405 | MET  |
| 1   | d     | 409 | ASN  |
| 1   | d     | 411 | ASP  |
| 1   | e     | 4   | THR  |
| 1   | e     | 17  | LEU  |
| 1   | e     | 20  | ASN  |
| 1   | e     | 31  | LYS  |
| 1   | e     | 54  | VAL  |
| 1   | e     | 95  | ASP  |
| 1   | e     | 98  | SER  |
| 1   | e     | 114 | LEU  |
| 1   | e     | 154 | THR  |
| 1   | e     | 157 | LEU  |
| 1   | e     | 158 | THR  |
| 1   | e     | 162 | LEU  |
| 1   | e     | 164 | LEU  |
| 1   | e     | 166 | SER  |
| 1   | e     | 186 | MET  |
| 1   | e     | 188 | LEU  |
| 1   | e     | 194 | SER  |
| 1   | e     | 224 | LYS  |
| 1   | e     | 228 | VAL  |
| 1   | e     | 245 | MET  |
| 1   | e     | 265 | ASP  |
| 1   | e     | 281 | SER  |
| 1   | e     | 286 | THR  |
| 1   | e     | 292 | ASN  |
| 1   | e     | 296 | ARG  |
| 1   | e     | 300 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | e     | 309 | GLU  |
| 1   | e     | 330 | VAL  |
| 1   | e     | 338 | THR  |
| 1   | e     | 346 | SER  |
| 1   | e     | 358 | ILE  |
| 1   | e     | 373 | THR  |
| 1   | e     | 374 | GLN  |
| 1   | e     | 375 | GLU  |
| 1   | e     | 376 | GLU  |
| 1   | e     | 382 | ILE  |
| 1   | e     | 383 | LEU  |
| 1   | e     | 390 | MET  |
| 1   | e     | 394 | ASP  |
| 1   | e     | 400 | ILE  |
| 1   | e     | 403 | LEU  |
| 1   | e     | 405 | MET  |
| 1   | e     | 409 | ASN  |
| 1   | e     | 411 | ASP  |
| 1   | f     | 4   | THR  |
| 1   | f     | 17  | LEU  |
| 1   | f     | 20  | ASN  |
| 1   | f     | 31  | LYS  |
| 1   | f     | 54  | VAL  |
| 1   | f     | 95  | ASP  |
| 1   | f     | 98  | SER  |
| 1   | f     | 114 | LEU  |
| 1   | f     | 154 | THR  |
| 1   | f     | 157 | LEU  |
| 1   | f     | 158 | THR  |
| 1   | f     | 162 | LEU  |
| 1   | f     | 164 | LEU  |
| 1   | f     | 166 | SER  |
| 1   | f     | 186 | MET  |
| 1   | f     | 188 | LEU  |
| 1   | f     | 194 | SER  |
| 1   | f     | 224 | LYS  |
| 1   | f     | 228 | VAL  |
| 1   | f     | 245 | MET  |
| 1   | f     | 265 | ASP  |
| 1   | f     | 281 | SER  |
| 1   | f     | 286 | THR  |
| 1   | f     | 292 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | f     | 296 | ARG  |
| 1   | f     | 300 | PHE  |
| 1   | f     | 309 | GLU  |
| 1   | f     | 330 | VAL  |
| 1   | f     | 338 | THR  |
| 1   | f     | 346 | SER  |
| 1   | f     | 358 | ILE  |
| 1   | f     | 373 | THR  |
| 1   | f     | 374 | GLN  |
| 1   | f     | 375 | GLU  |
| 1   | f     | 376 | GLU  |
| 1   | f     | 382 | ILE  |
| 1   | f     | 383 | LEU  |
| 1   | f     | 390 | MET  |
| 1   | f     | 394 | ASP  |
| 1   | f     | 400 | ILE  |
| 1   | f     | 403 | LEU  |
| 1   | f     | 405 | MET  |
| 1   | f     | 409 | ASN  |
| 1   | f     | 411 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a     | 20  | ASN  |
| 1   | a     | 32  | GLN  |
| 1   | a     | 126 | ASN  |
| 1   | a     | 295 | HIS  |
| 1   | b     | 32  | GLN  |
| 1   | b     | 126 | ASN  |
| 1   | b     | 295 | HIS  |
| 1   | b     | 388 | HIS  |
| 1   | c     | 20  | ASN  |
| 1   | c     | 32  | GLN  |
| 1   | c     | 126 | ASN  |
| 1   | c     | 295 | HIS  |
| 1   | d     | 32  | GLN  |
| 1   | d     | 90  | ASN  |
| 1   | d     | 126 | ASN  |
| 1   | d     | 193 | GLN  |
| 1   | e     | 20  | ASN  |
| 1   | e     | 32  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | e     | 126  | ASN  |
| 1   | e     | 295  | HIS  |
| 1   | e     | 388  | HIS  |
| 1   | f     | 32   | GLN  |
| 1   | f     | 126  | ASN  |
| 1   | f     | 193  | GLN  |
| 1   | f     | 295  | HIS  |
| 2   | A     | 14   | ASN  |
| 2   | A     | 48   | GLN  |
| 2   | A     | 129  | GLN  |
| 2   | A     | 157  | ASN  |
| 2   | A     | 286  | ASN  |
| 2   | A     | 303  | HIS  |
| 2   | A     | 321  | ASN  |
| 2   | A     | 353  | HIS  |
| 2   | A     | 412  | ASN  |
| 3   | U     | 41   | ASN  |
| 3   | U     | 227  | GLN  |
| 3   | V     | 37   | HIS  |
| 5   | X     | 193  | ASN  |
| 5   | X     | 513  | GLN  |
| 5   | X     | 517  | GLN  |
| 5   | X     | 684  | ASN  |
| 5   | X     | 688  | GLN  |
| 5   | X     | 798  | GLN  |
| 5   | X     | 799  | ASN  |
| 5   | X     | 932  | GLN  |
| 5   | X     | 1116 | HIS  |
| 5   | X     | 1268 | GLN  |
| 6   | Y     | 320  | ASN  |
| 6   | Y     | 365  | GLN  |
| 6   | Y     | 448  | GLN  |
| 6   | Y     | 458  | ASN  |
| 6   | Y     | 477  | GLN  |
| 6   | Y     | 488  | ASN  |
| 6   | Y     | 669  | GLN  |
| 6   | Y     | 690  | ASN  |
| 6   | Y     | 716  | GLN  |
| 6   | Y     | 739  | GLN  |
| 6   | Y     | 1044 | GLN  |
| 6   | Y     | 1108 | GLN  |
| 6   | Y     | 1268 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 6   | Y     | 1289 | ASN  |
| 6   | Y     | 1295 | ASN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 9   | R     | 15/99 (15%) | 1 (6%)            | 0               |

All (1) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | R     | 91  | G    |

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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 | $\# Z  > 2$ |
| 10  | BEF  | d     | 1002 | -    | 0,3,3        | -    | -           | -           |      |             |
| 10  | BEF  | c     | 1002 | -    | 0,3,3        | -    | -           | -           |      |             |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | ADP  | f     | 1000 | 1    | 27,29,29     | 1.37 | 4 (14%)  | 42,45,45    | 1.96 | 10 (23%) |
| 10  | BEF  | b     | 501  | -    | 0,3,3        | -    | -        | -           |      |          |
| 10  | BEF  | e     | 1002 | -    | 0,3,3        | -    | -        | -           |      |          |
| 11  | ADP  | c     | 1000 | 12,1 | 27,29,29     | 1.36 | 4 (14%)  | 42,45,45    | 1.96 | 11 (26%) |
| 11  | ADP  | e     | 1000 | 12   | 27,29,29     | 1.36 | 4 (14%)  | 42,45,45    | 1.96 | 10 (23%) |
| 11  | ADP  | d     | 1000 | 12,1 | 27,29,29     | 1.37 | 4 (14%)  | 42,45,45    | 1.98 | 10 (23%) |
| 10  | BEF  | f     | 1002 | -    | 0,3,3        | -    | -        | -           |      |          |
| 11  | ADP  | b     | 502  | 12,1 | 27,29,29     | 1.36 | 4 (14%)  | 42,45,45    | 1.98 | 9 (21%)  |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 11  | ADP  | f     | 1000 | 1    | -       | 2/16/32/32 | 0/3/3/3 |
| 11  | ADP  | b     | 502  | 12,1 | -       | 6/16/32/32 | 0/3/3/3 |
| 11  | ADP  | c     | 1000 | 12,1 | -       | 1/16/32/32 | 0/3/3/3 |
| 11  | ADP  | d     | 1000 | 12,1 | -       | 1/16/32/32 | 0/3/3/3 |
| 11  | ADP  | e     | 1000 | 12   | -       | 1/16/32/32 | 0/3/3/3 |

All (20) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | b     | 502  | ADP  | C5-C4 | 4.65  | 1.47        | 1.39     |
| 11  | f     | 1000 | ADP  | C5-C4 | 4.62  | 1.47        | 1.39     |
| 11  | d     | 1000 | ADP  | C5-C4 | 4.58  | 1.47        | 1.39     |
| 11  | e     | 1000 | ADP  | C5-C4 | 4.57  | 1.47        | 1.39     |
| 11  | c     | 1000 | ADP  | C5-C4 | 4.55  | 1.47        | 1.39     |
| 11  | d     | 1000 | ADP  | C5-C6 | 2.74  | 1.48        | 1.41     |
| 11  | e     | 1000 | ADP  | C5-C6 | 2.71  | 1.48        | 1.41     |
| 11  | c     | 1000 | ADP  | C5-C6 | 2.70  | 1.48        | 1.41     |
| 11  | f     | 1000 | ADP  | C5-C6 | 2.67  | 1.48        | 1.41     |
| 11  | b     | 502  | ADP  | C5-C6 | 2.65  | 1.48        | 1.41     |
| 11  | c     | 1000 | ADP  | C8-N7 | 2.49  | 1.36        | 1.31     |
| 11  | e     | 1000 | ADP  | C8-N7 | 2.46  | 1.36        | 1.31     |
| 11  | d     | 1000 | ADP  | C8-N7 | 2.44  | 1.36        | 1.31     |
| 11  | f     | 1000 | ADP  | C8-N7 | 2.39  | 1.36        | 1.31     |
| 11  | b     | 502  | ADP  | C8-N7 | 2.28  | 1.35        | 1.31     |
| 11  | f     | 1000 | ADP  | C5-N7 | -2.17 | 1.34        | 1.39     |
| 11  | b     | 502  | ADP  | C5-N7 | -2.16 | 1.34        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | e     | 1000 | ADP  | C5-N7 | -2.15 | 1.34        | 1.39     |
| 11  | d     | 1000 | ADP  | C5-N7 | -2.14 | 1.35        | 1.39     |
| 11  | c     | 1000 | ADP  | C5-N7 | -2.09 | 1.35        | 1.39     |

All (50) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | b     | 502  | ADP  | C5-C4-N3    | -6.36 | 118.46      | 126.75   |
| 11  | f     | 1000 | ADP  | C5-C4-N3    | -6.28 | 118.56      | 126.75   |
| 11  | e     | 1000 | ADP  | C5-C4-N3    | -6.24 | 118.61      | 126.75   |
| 11  | d     | 1000 | ADP  | C5-C4-N3    | -6.19 | 118.68      | 126.75   |
| 11  | c     | 1000 | ADP  | C5-C4-N3    | -6.04 | 118.87      | 126.75   |
| 11  | b     | 502  | ADP  | N3-C4-N9    | 5.08  | 135.46      | 127.08   |
| 11  | f     | 1000 | ADP  | N3-C4-N9    | 4.94  | 135.22      | 127.08   |
| 11  | e     | 1000 | ADP  | N3-C4-N9    | 4.84  | 135.06      | 127.08   |
| 11  | d     | 1000 | ADP  | N3-C4-N9    | 4.82  | 135.03      | 127.08   |
| 11  | c     | 1000 | ADP  | N3-C4-N9    | 4.70  | 134.83      | 127.08   |
| 11  | d     | 1000 | ADP  | C2-N3-C4    | 3.86  | 120.86      | 111.75   |
| 11  | f     | 1000 | ADP  | C2-N3-C4    | 3.86  | 120.86      | 111.75   |
| 11  | e     | 1000 | ADP  | C2-N3-C4    | 3.85  | 120.86      | 111.75   |
| 11  | b     | 502  | ADP  | C2-N3-C4    | 3.83  | 120.79      | 111.75   |
| 11  | c     | 1000 | ADP  | C2-N3-C4    | 3.81  | 120.76      | 111.75   |
| 11  | d     | 1000 | ADP  | PA-O3A-PB   | -3.36 | 121.29      | 132.83   |
| 11  | d     | 1000 | ADP  | C4-C5-N7    | -3.27 | 106.64      | 110.62   |
| 11  | c     | 1000 | ADP  | PA-O3A-PB   | -3.26 | 121.63      | 132.83   |
| 11  | c     | 1000 | ADP  | C4-C5-N7    | -3.26 | 106.65      | 110.62   |
| 11  | f     | 1000 | ADP  | C4-C5-N7    | -3.25 | 106.66      | 110.62   |
| 11  | e     | 1000 | ADP  | C4-C5-N7    | -3.24 | 106.67      | 110.62   |
| 11  | b     | 502  | ADP  | C4-C5-N7    | -3.19 | 106.74      | 110.62   |
| 11  | e     | 1000 | ADP  | PA-O3A-PB   | -3.17 | 121.96      | 132.83   |
| 11  | c     | 1000 | ADP  | N3-C2-N1    | -3.13 | 123.71      | 128.60   |
| 11  | d     | 1000 | ADP  | N3-C2-N1    | -3.12 | 123.73      | 128.60   |
| 11  | f     | 1000 | ADP  | N3-C2-N1    | -3.10 | 123.75      | 128.60   |
| 11  | e     | 1000 | ADP  | N3-C2-N1    | -3.08 | 123.78      | 128.60   |
| 11  | b     | 502  | ADP  | PA-O3A-PB   | -3.04 | 122.39      | 132.83   |
| 11  | f     | 1000 | ADP  | PA-O3A-PB   | -3.03 | 122.42      | 132.83   |
| 11  | b     | 502  | ADP  | N3-C2-N1    | -3.03 | 123.86      | 128.60   |
| 11  | f     | 1000 | ADP  | C5-N7-C8    | 2.75  | 107.42      | 103.51   |
| 11  | d     | 1000 | ADP  | C5-N7-C8    | 2.74  | 107.41      | 103.51   |
| 11  | c     | 1000 | ADP  | C5-N7-C8    | 2.74  | 107.40      | 103.51   |
| 11  | e     | 1000 | ADP  | C5-N7-C8    | 2.71  | 107.36      | 103.51   |
| 11  | e     | 1000 | ADP  | C3'-C2'-C1' | 2.67  | 106.50      | 101.43   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | b     | 502  | ADP  | C5-N7-C8    | 2.62  | 107.23      | 103.51   |
| 11  | c     | 1000 | ADP  | C4-N9-C8    | 2.62  | 108.57      | 105.73   |
| 11  | c     | 1000 | ADP  | C3'-C2'-C1' | 2.62  | 106.40      | 101.43   |
| 11  | d     | 1000 | ADP  | C3'-C2'-C1' | 2.58  | 106.32      | 101.43   |
| 11  | f     | 1000 | ADP  | C4-N9-C8    | 2.55  | 108.49      | 105.73   |
| 11  | b     | 502  | ADP  | C3'-C2'-C1' | 2.55  | 106.27      | 101.43   |
| 11  | d     | 1000 | ADP  | C4-N9-C8    | 2.54  | 108.48      | 105.73   |
| 11  | f     | 1000 | ADP  | C3'-C2'-C1' | 2.51  | 106.19      | 101.43   |
| 11  | b     | 502  | ADP  | C4-N9-C8    | 2.49  | 108.42      | 105.73   |
| 11  | e     | 1000 | ADP  | C4-N9-C8    | 2.42  | 108.35      | 105.73   |
| 11  | c     | 1000 | ADP  | C6-C5-N7    | 2.23  | 136.18      | 132.02   |
| 11  | d     | 1000 | ADP  | C6-C5-N7    | 2.17  | 136.07      | 132.02   |
| 11  | f     | 1000 | ADP  | C6-C5-N7    | 2.12  | 135.97      | 132.02   |
| 11  | e     | 1000 | ADP  | C6-C5-N7    | 2.11  | 135.96      | 132.02   |
| 11  | c     | 1000 | ADP  | N9-C8-N7    | -2.07 | 111.08      | 113.91   |

There are no chirality outliers.

All (11) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 11  | b     | 502  | ADP  | C5'-O5'-PA-O2A  |
| 11  | b     | 502  | ADP  | C5'-O5'-PA-O3A  |
| 11  | f     | 1000 | ADP  | O4'-C4'-C5'-O5' |
| 11  | b     | 502  | ADP  | PB-O3A-PA-O1A   |
| 11  | b     | 502  | ADP  | O4'-C4'-C5'-O5' |
| 11  | f     | 1000 | ADP  | PB-O3A-PA-O2A   |
| 11  | b     | 502  | ADP  | C5'-O5'-PA-O1A  |
| 11  | b     | 502  | ADP  | PB-O3A-PA-O2A   |
| 11  | d     | 1000 | ADP  | O4'-C4'-C5'-O5' |
| 11  | e     | 1000 | ADP  | O4'-C4'-C5'-O5' |
| 11  | c     | 1000 | ADP  | O4'-C4'-C5'-O5' |

There are no ring outliers.

6 monomers are involved in 5 short contacts:

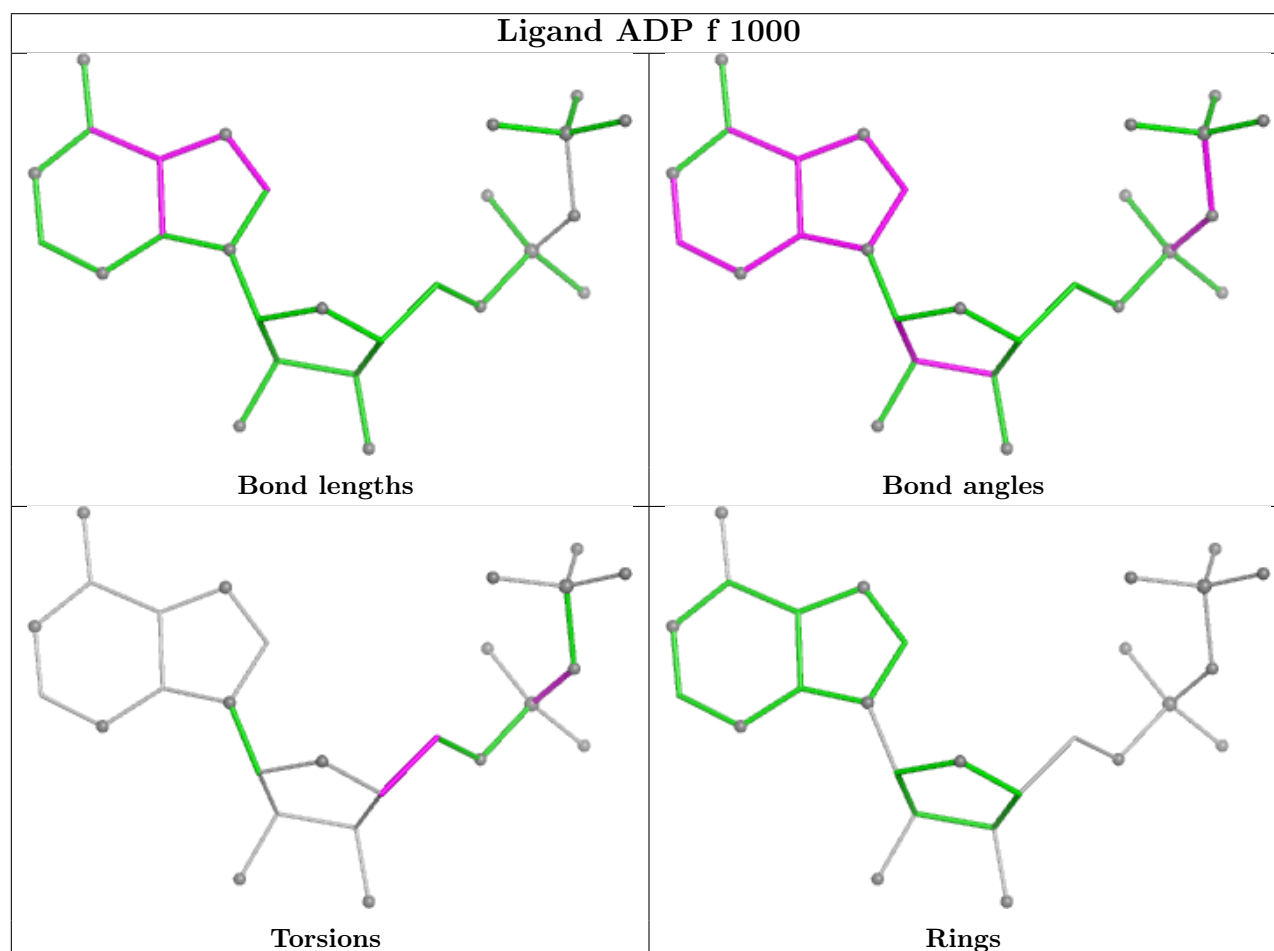
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 10  | d     | 1002 | BEF  | 1       | 0            |
| 11  | f     | 1000 | ADP  | 1       | 0            |
| 10  | e     | 1002 | BEF  | 1       | 0            |
| 11  | e     | 1000 | ADP  | 1       | 0            |
| 11  | d     | 1000 | ADP  | 1       | 0            |

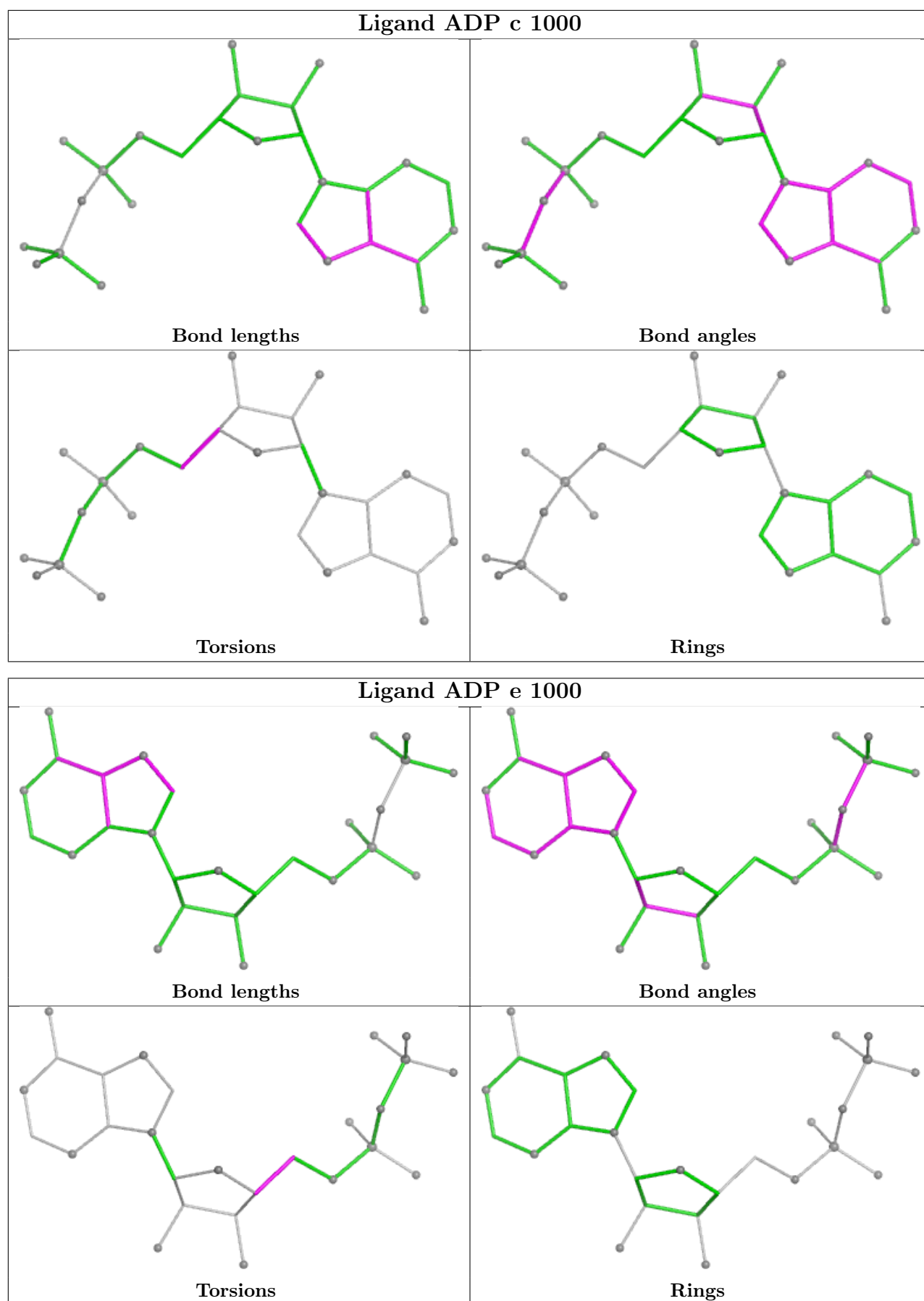
*Continued on next page...*

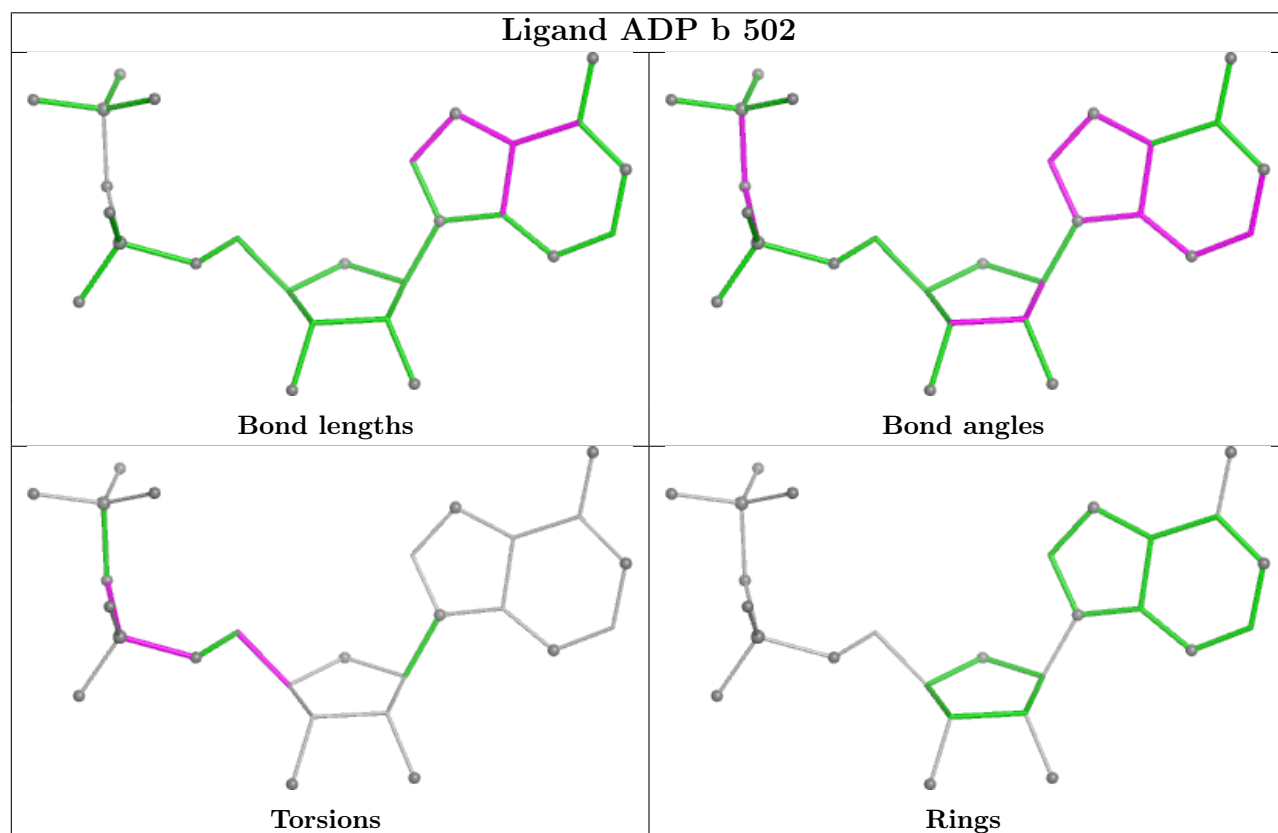
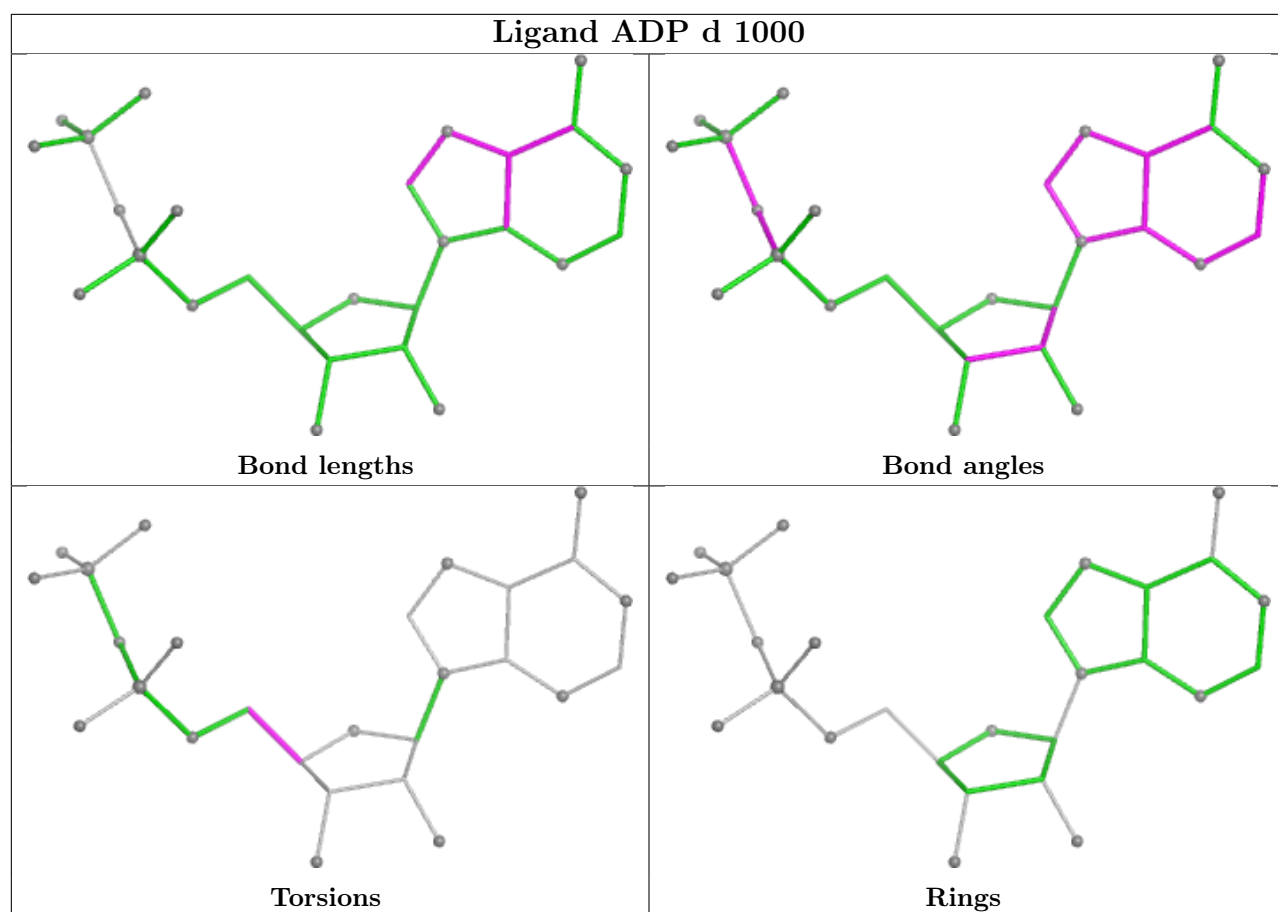
*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 11  | b     | 502 | ADP  | 2       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

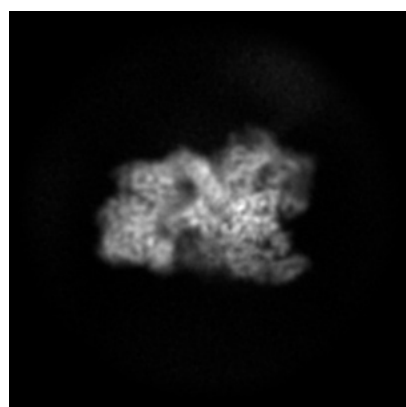
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11722. These allow visual inspection of the internal detail of the map and identification of artifacts.

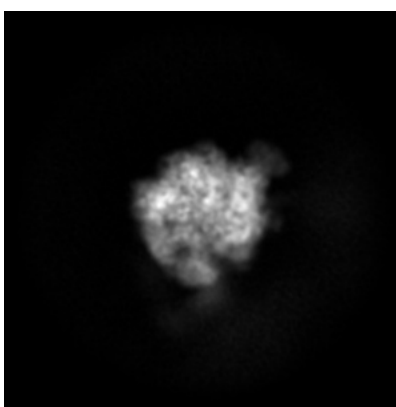
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

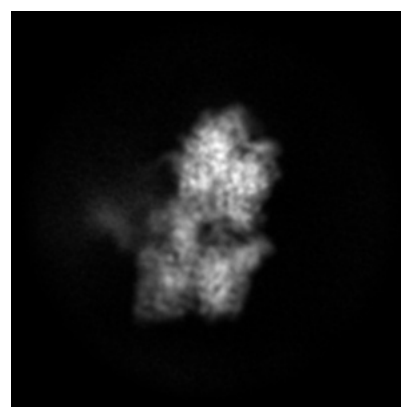
#### 6.1.1 Primary map



X



Y

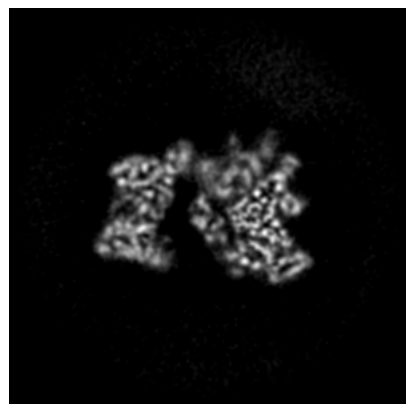


Z

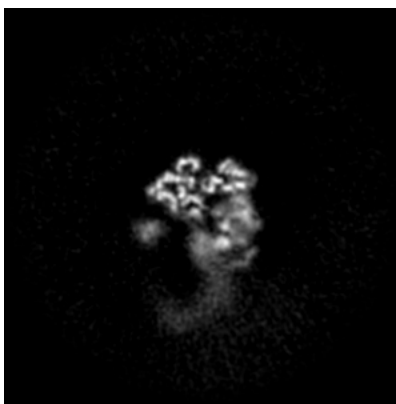
The images above show the map projected in three orthogonal directions.

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

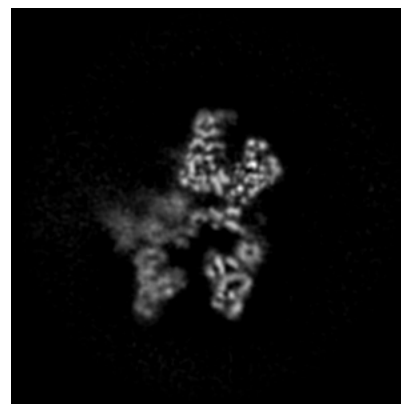
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

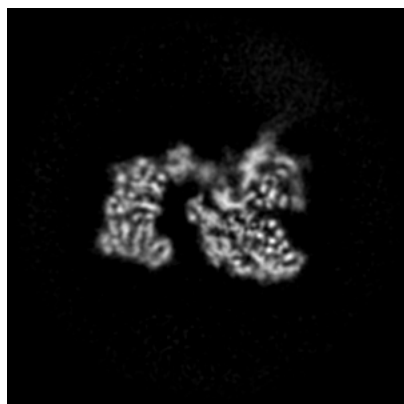


Z Index: 150

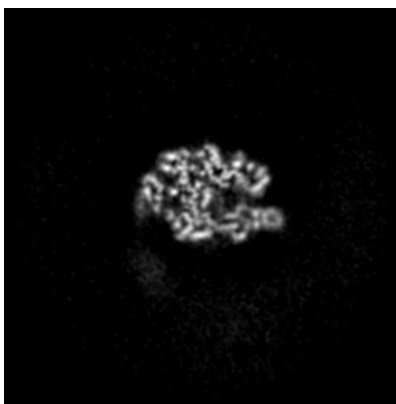
The images above show central slices of the map in three orthogonal directions.

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

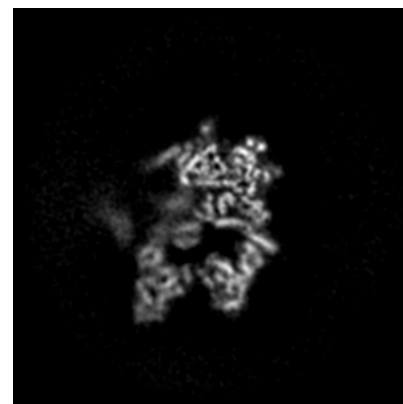
### 6.3.1 Primary map



X Index: 156



Y Index: 169

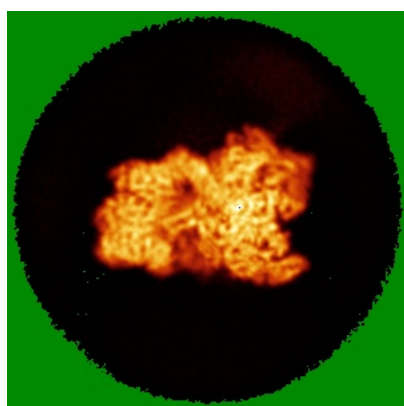


Z Index: 143

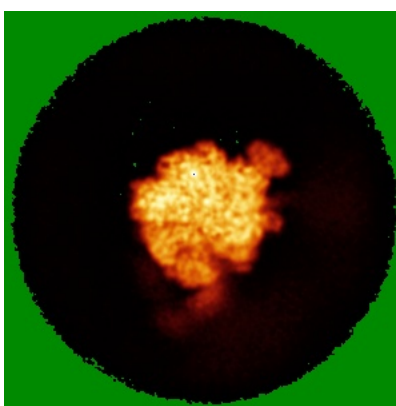
The images above show the largest variance slices of the map in three orthogonal directions.

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

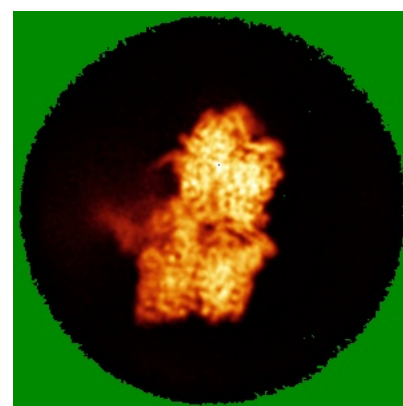
### 6.4.1 Primary map



X



Y

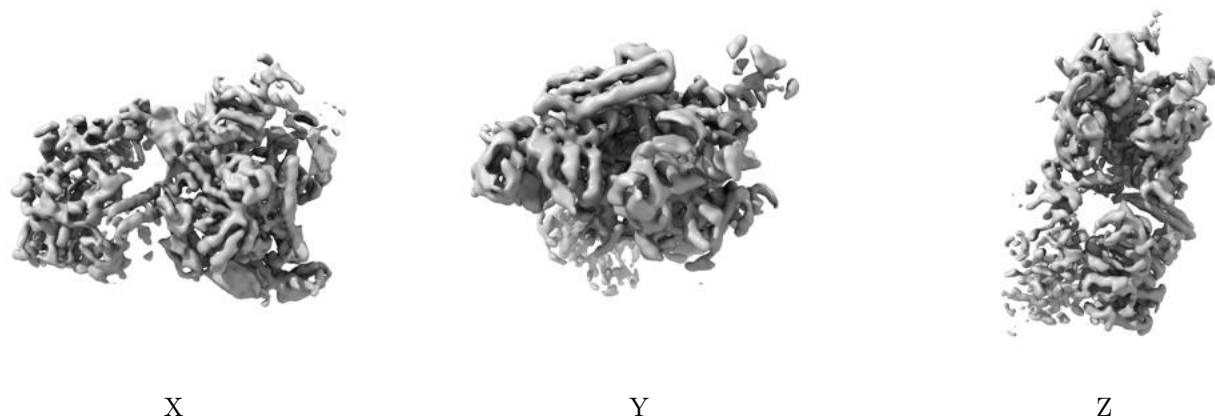


Z

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.

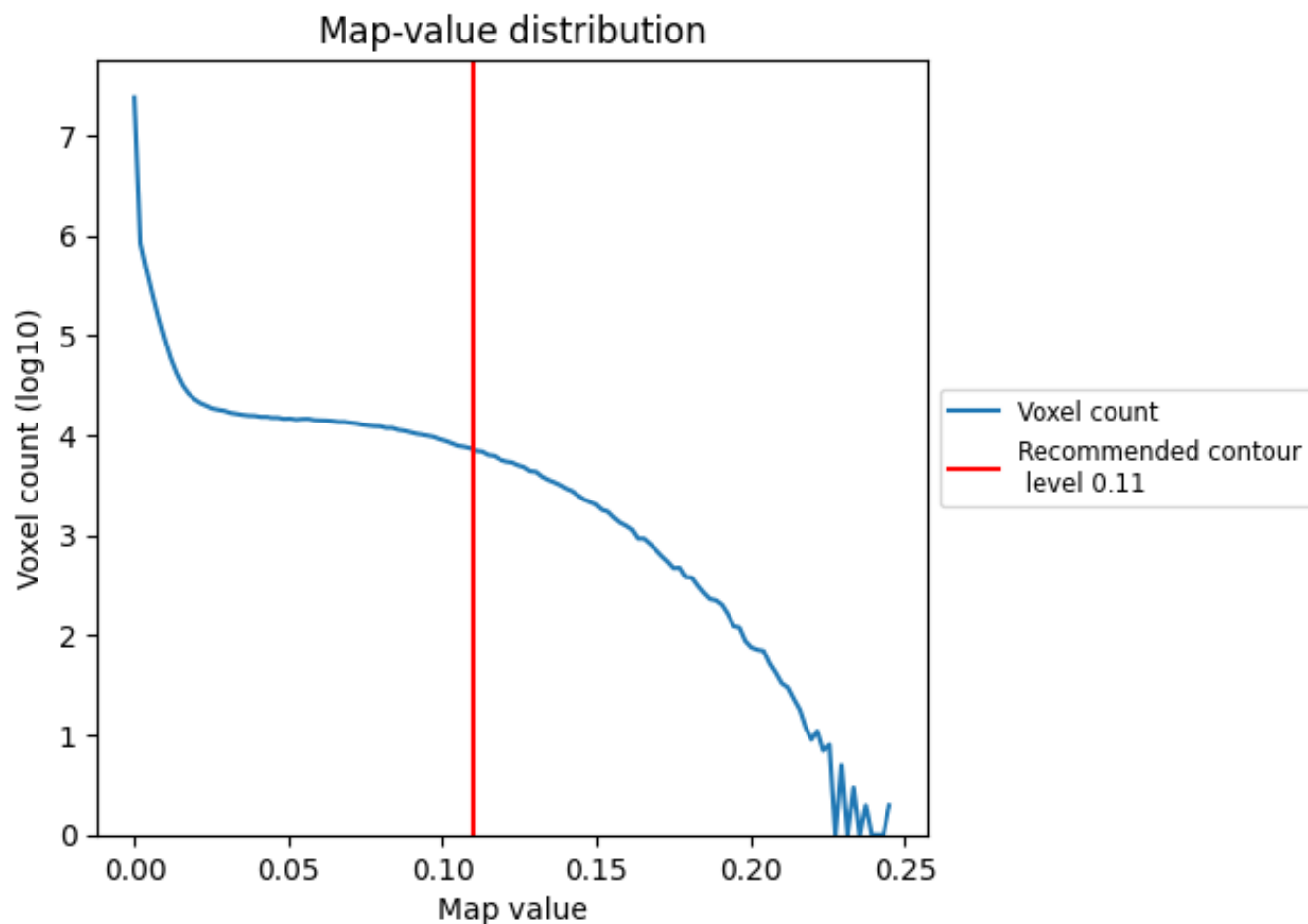
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

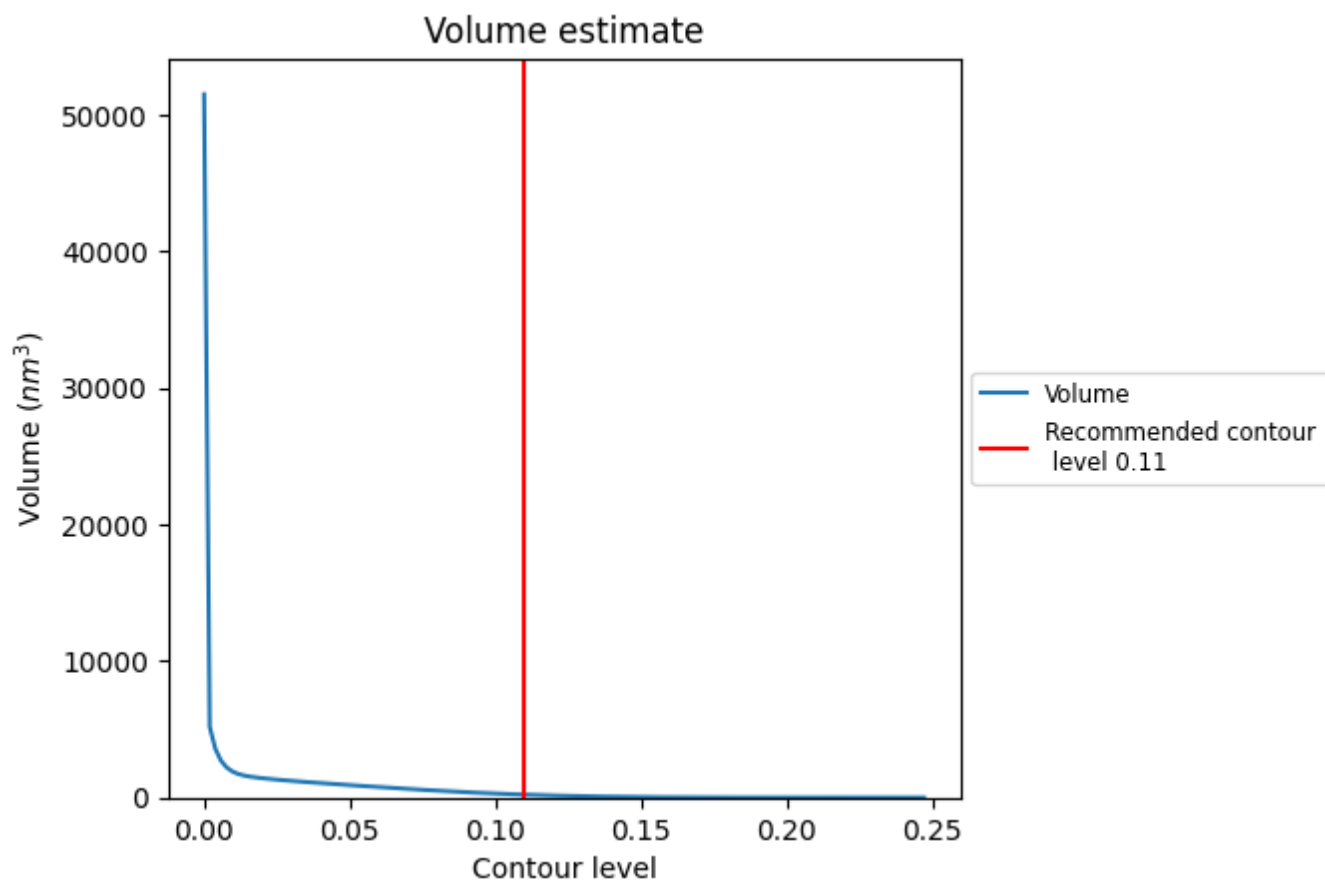
This section contains the results of statistical analysis of the map.

### 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.

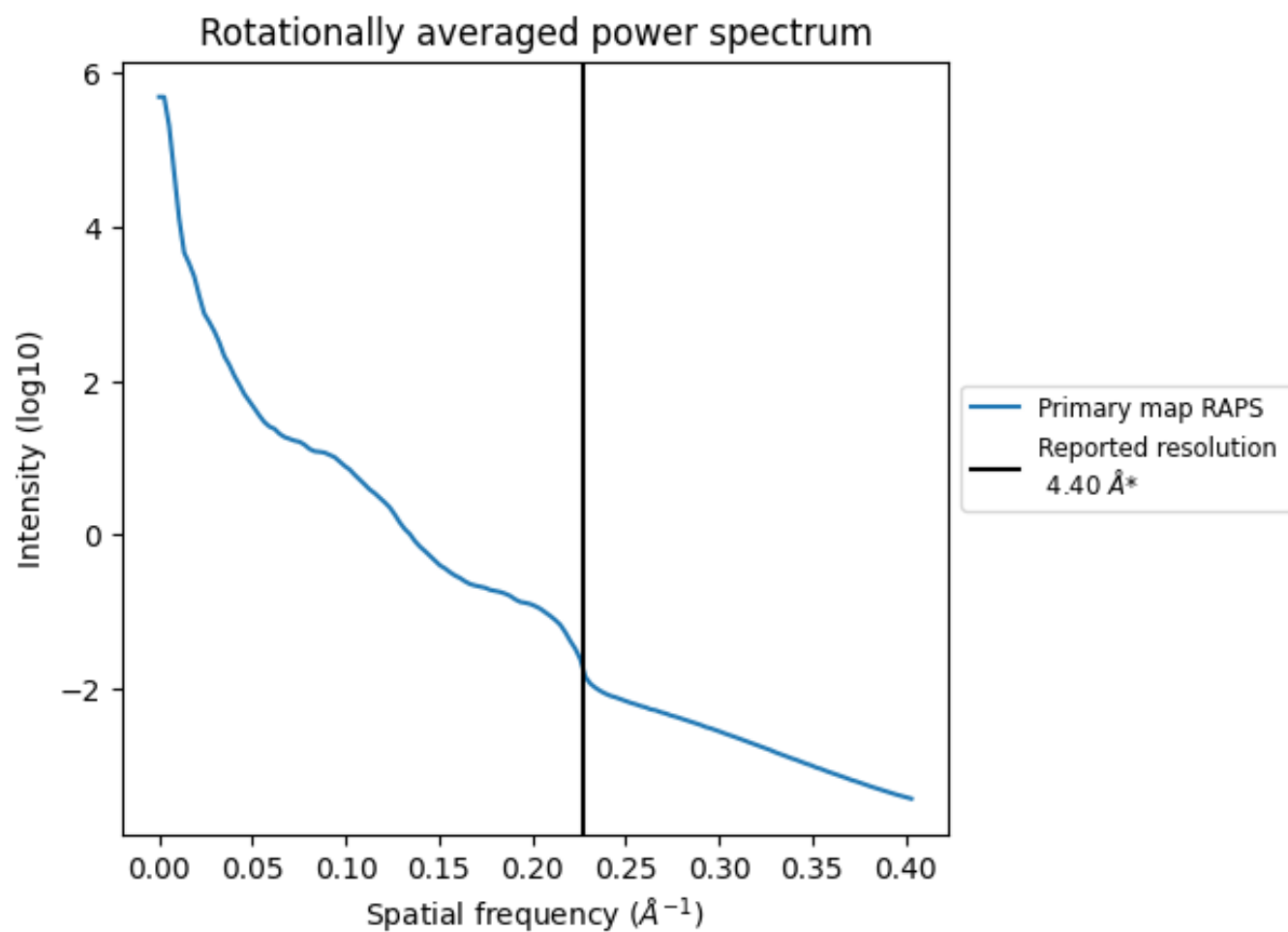
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 212 nm<sup>3</sup>; this corresponds to an approximate mass of 191 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 ⓘ

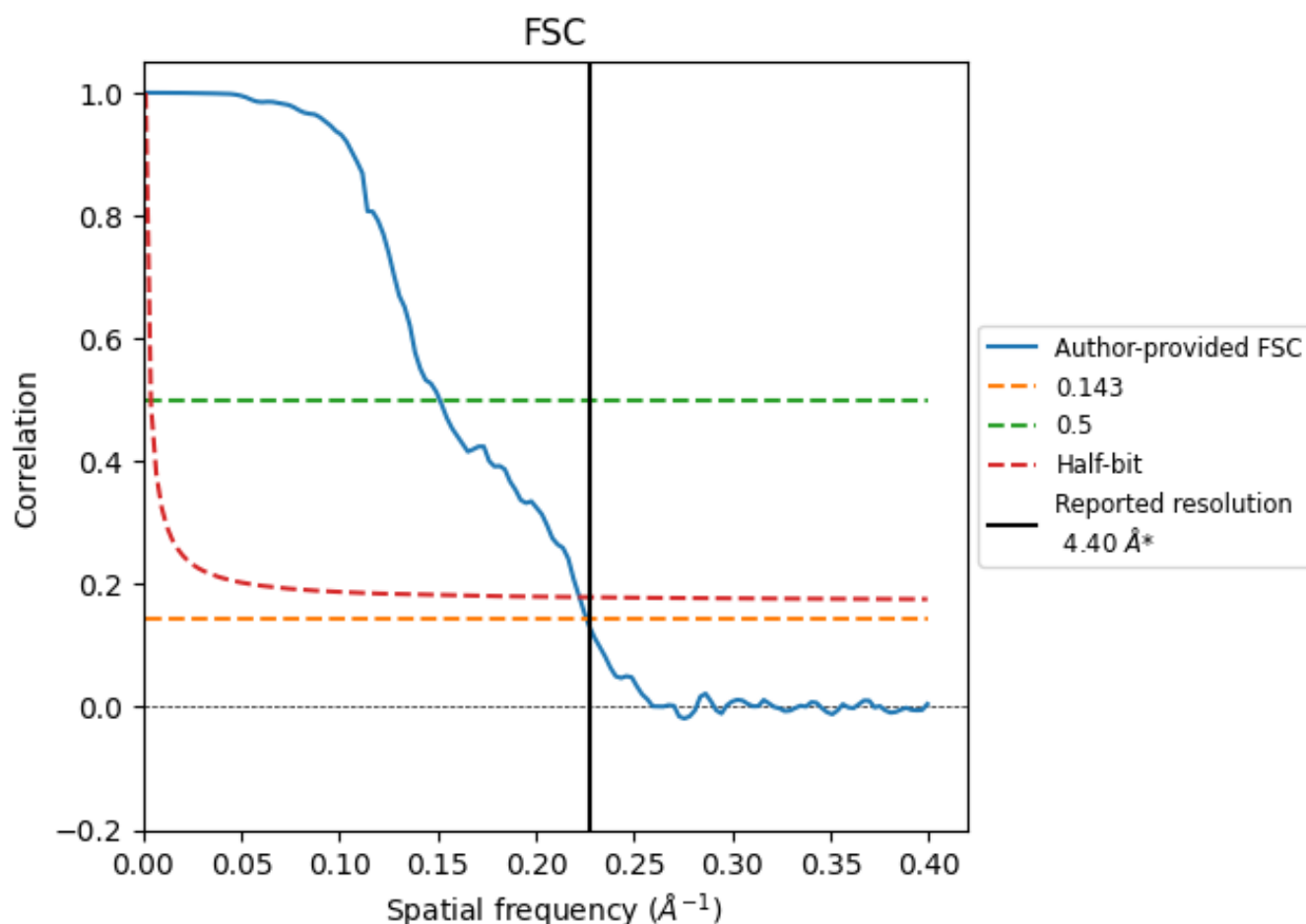


\*Reported resolution corresponds to spatial frequency of 0.227 Å<sup>-1</sup>

## 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 0.227 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

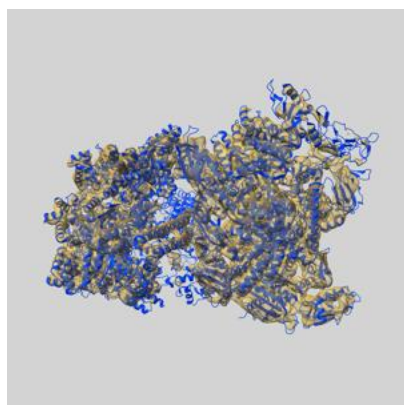
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.40                               | -    | -        |
| Author-provided FSC curve | 4.43                               | 6.63 | 4.50     |
| Unmasked-calculated*      | -                                  | -    | -        |

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

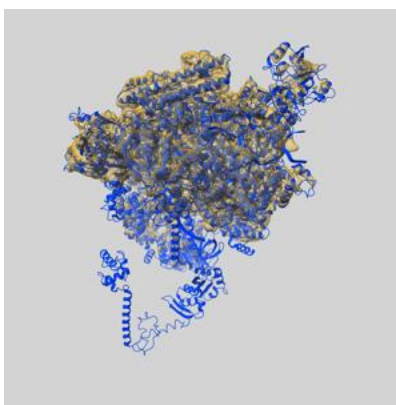
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11722 and PDB model 7ADB. Per-residue inclusion information can be found in section [3](#) on page [10](#).

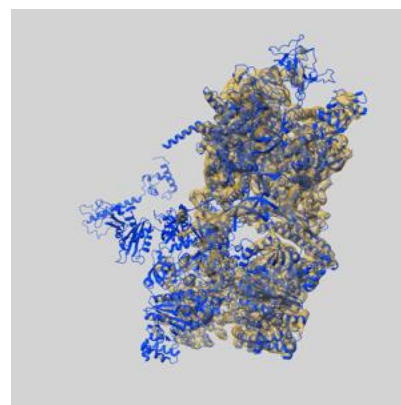
### 9.1 Map-model overlay [i](#)



X



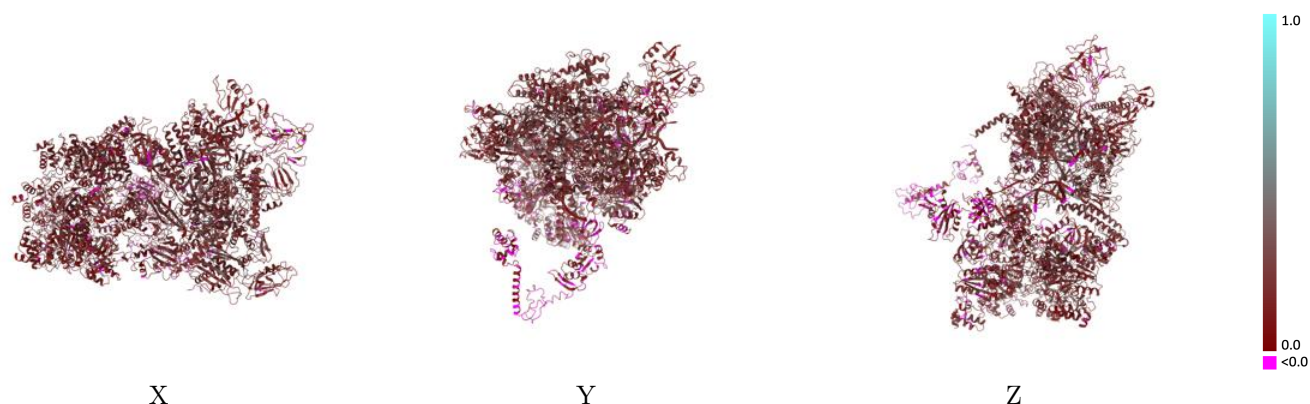
Y



Z

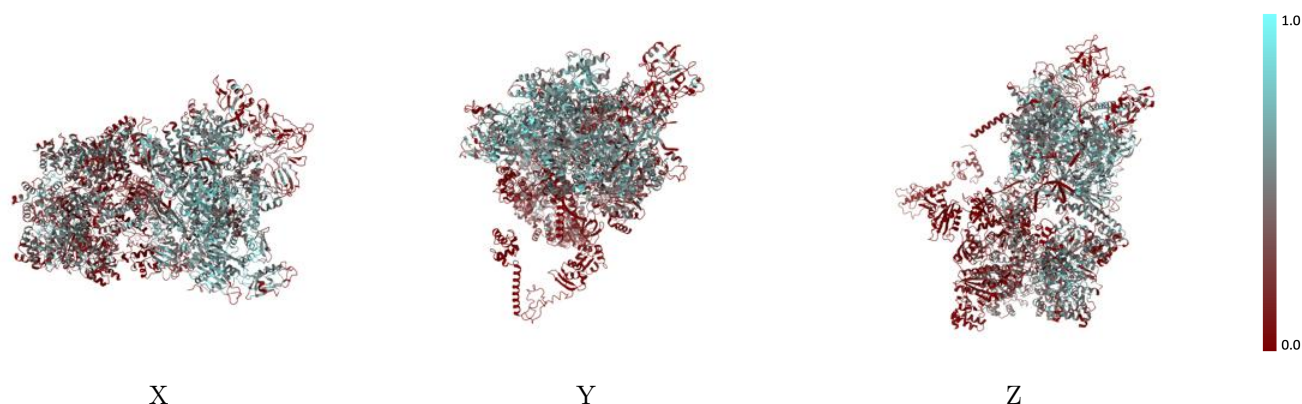
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



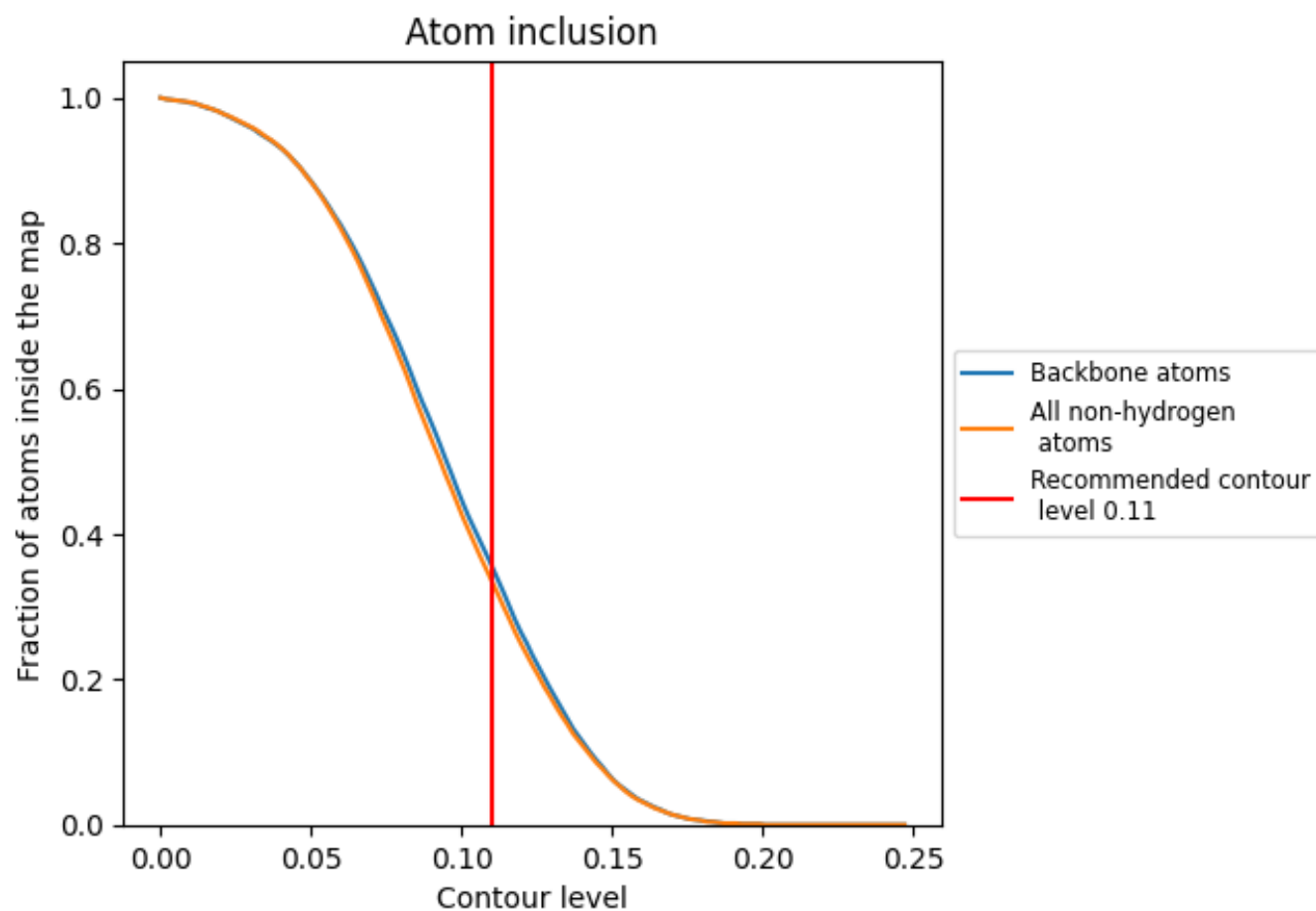
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 36% of all backbone atoms, 34% 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> 0.3350 | <div></div> 0.1860 |
| A     | <div></div> 0.0130 | <div></div> 0.0780 |
| K     | <div></div> 0.2640 | <div></div> 0.1400 |
| L     | <div></div> 0.5250 | <div></div> 0.2030 |
| R     | <div></div> 0.4010 | <div></div> 0.1810 |
| U     | <div></div> 0.3600 | <div></div> 0.1990 |
| V     | <div></div> 0.4600 | <div></div> 0.2070 |
| W     | <div></div> 0.1260 | <div></div> 0.2140 |
| X     | <div></div> 0.4730 | <div></div> 0.2240 |
| Y     | <div></div> 0.4170 | <div></div> 0.2040 |
| a     | <div></div> 0.2260 | <div></div> 0.1670 |
| b     | <div></div> 0.3780 | <div></div> 0.1860 |
| c     | <div></div> 0.4020 | <div></div> 0.1840 |
| d     | <div></div> 0.3660 | <div></div> 0.1820 |
| e     | <div></div> 0.2430 | <div></div> 0.1620 |
| f     | <div></div> 0.0860 | <div></div> 0.1520 |

1.0

0.0

<0.0