



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:07 PM UTC

PDB ID : 8E70 / pdb\_00008e70  
EMDB ID : EMD-27932  
Title : Escherichia coli Rho-dependent transcription pre-termination complex containing 18 nt long RNA spacer, dC75 rut mimic RNA, Mg-ADP-BeF<sub>3</sub>, and NusG; Rho hexamer part  
Authors : Molodtsov, V.; Wang, C.; Ebright, R.H.  
Deposited on : 2022-08-23  
Resolution : 4.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

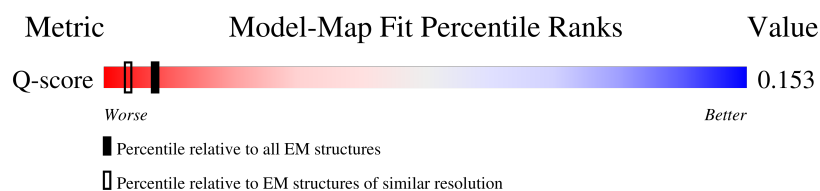
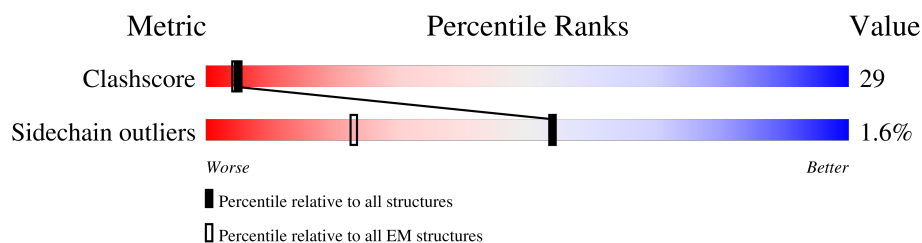
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 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                       | -                                                        |
| Sidechain outliers | 223484                      | 23102                       | -                                                        |
| Q-score            | -                           | 25397                       | 6458 ( 3.60 - 4.60 )                                     |

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   | 8     | 79     |                  |
| 2   | a     | 419    |                  |
| 2   | b     | 419    |                  |
| 2   | c     | 419    |                  |
| 2   | d     | 419    |                  |

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| Mol | Chain | Length | Quality of chain                                                                           |
|-----|-------|--------|--------------------------------------------------------------------------------------------|
| 2   | e     | 419    |  80% 18% |
| 2   | f     | 419    |  79% 20% |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3   | ADP  | a     | 1000 | -         | -        | X       | -                |
| 3   | ADP  | b     | 1000 | -         | -        | X       | -                |
| 3   | ADP  | c     | 1000 | -         | -        | X       | -                |
| 3   | ADP  | d     | 1000 | -         | -        | X       | -                |
| 3   | ADP  | e     | 1000 | -         | -        | X       | -                |
| 3   | ADP  | f     | 1000 | -         | -        | X       | -                |
| 5   | BEF  | a     | 1002 | -         | -        | X       | -                |
| 5   | BEF  | b     | 1002 | -         | -        | X       | -                |
| 5   | BEF  | c     | 1002 | -         | -        | X       | -                |
| 5   | BEF  | d     | 1002 | -         | -        | X       | -                |
| 5   | BEF  | e     | 1002 | -         | -        | X       | -                |
| 5   | BEF  | f     | 1002 | -         | -        | X       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21097 atoms, of which 63 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 DNA chain called dC75 RNA.

| Mol | Chain | Residues | Atoms |     |    |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|-----|----|---------|-------|
| 1   | 8     | 61       | Total | C   | H  | N   | O   | P  | 0       | 0     |
|     |       |          | 1225  | 552 | 63 | 180 | 369 | 61 |         |       |

- Molecule 2 is a protein called Transcription termination factor Rho.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | e     | 417      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3280  | 2065 | 581 | 617 | 17 |         |       |
| 2   | f     | 417      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3280  | 2065 | 581 | 617 | 17 |         |       |
| 2   | c     | 417      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3280  | 2065 | 581 | 617 | 17 |         |       |
| 2   | b     | 417      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3280  | 2065 | 581 | 617 | 17 |         |       |
| 2   | a     | 417      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3280  | 2065 | 581 | 617 | 17 |         |       |
| 2   | d     | 417      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3280  | 2065 | 581 | 617 | 17 |         |       |

- Molecule 3 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>).

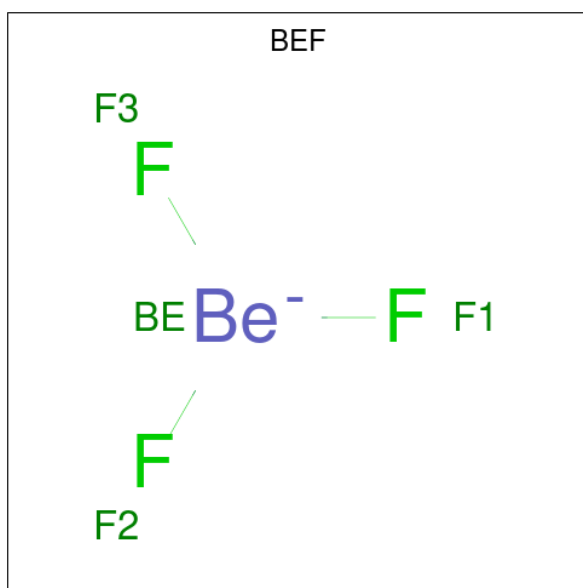


| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 3   | e     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 3   | f     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 3   | c     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 3   | b     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 3   | a     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 3   | d     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 4   | e     | 1        | Total Mg<br>1 1 | 0       |
| 4   | f     | 1        | Total Mg<br>1 1 | 0       |
| 4   | c     | 1        | Total Mg<br>1 1 | 0       |
| 4   | b     | 1        | Total Mg<br>1 1 | 0       |
| 4   | a     | 1        | Total Mg<br>1 1 | 0       |
| 4   | d     | 1        | Total Mg<br>1 1 | 0       |

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula:  $\text{BeF}_3$ ).

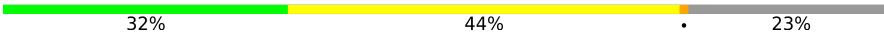


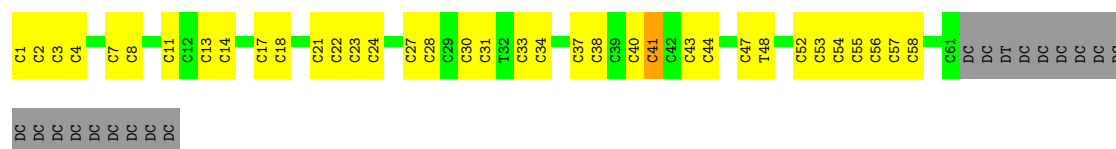
| Mol | Chain | Residues | Atoms      |         |        | AltConf |
|-----|-------|----------|------------|---------|--------|---------|
| 5   | e     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |
| 5   | f     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |
| 5   | c     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |
| 5   | b     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |
| 5   | a     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |
| 5   | d     | 1        | Total<br>4 | Be<br>1 | F<br>3 | 0       |

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

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.

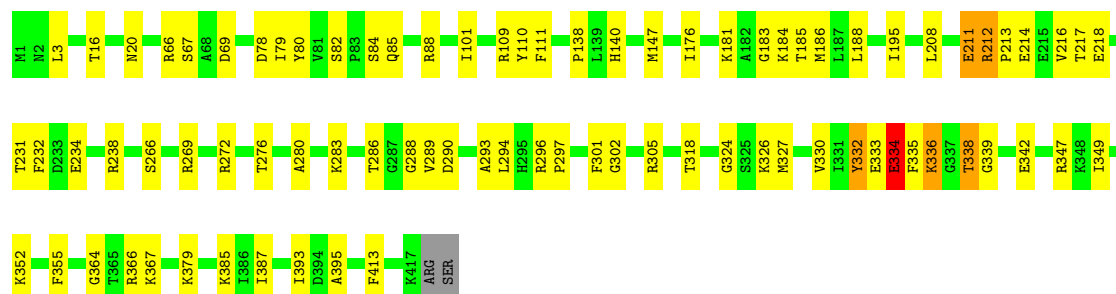
- Molecule 1: dC75 RNA

Chain 8: 



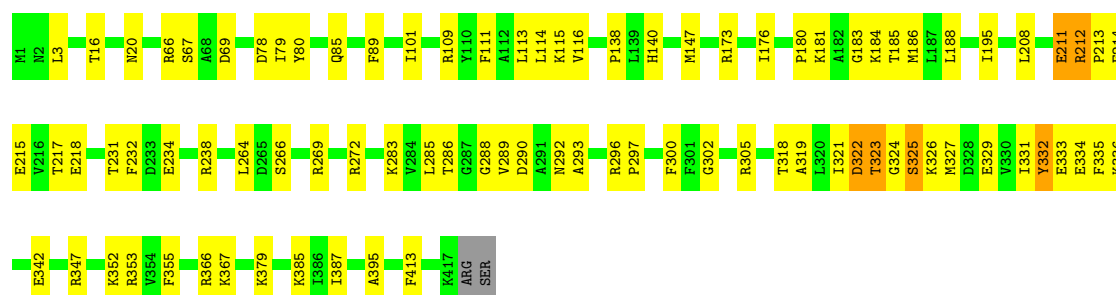
- Molecule 2: Transcription termination factor Rho

Chain e: 



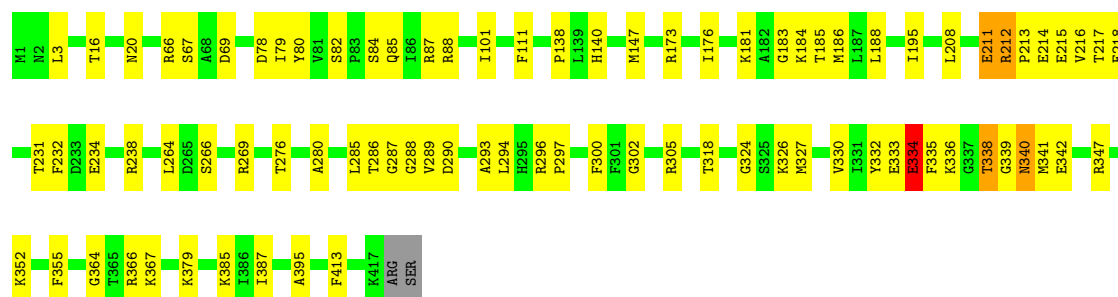
- Molecule 2: Transcription termination factor Rho

Chain f: 



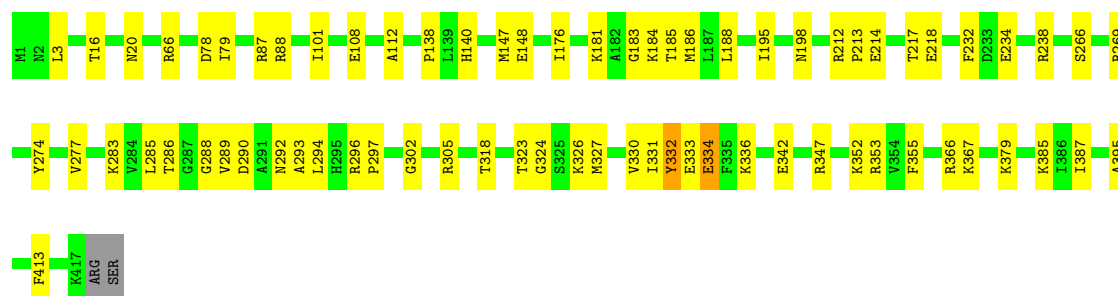
- Molecule 2: Transcription termination factor Rho

Chain c:  79% 19%



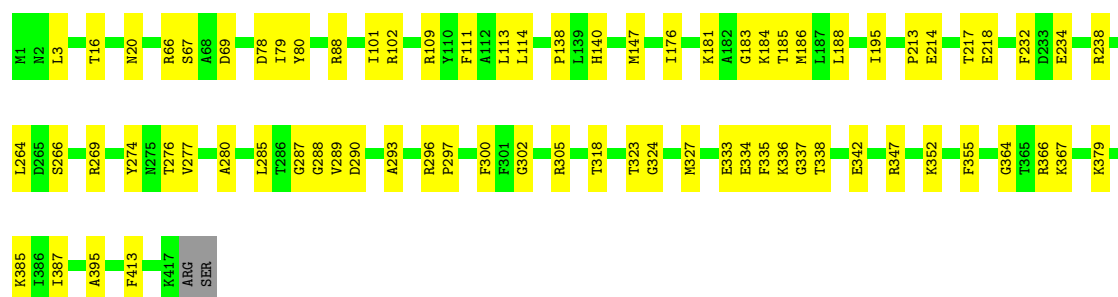
• Molecule 2: Transcription termination factor Rho

Chain b:  82% 17%



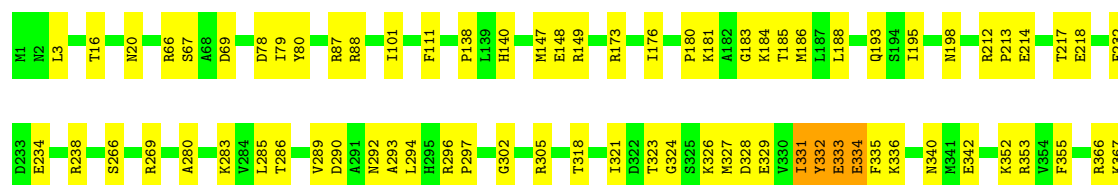
• Molecule 2: Transcription termination factor Rho

Chain a:  82% 18%



• Molecule 2: Transcription termination factor Rho

Chain d:  81% 18%



|      |      |      |      |      |      |      |     |     |
|------|------|------|------|------|------|------|-----|-----|
| K379 | K385 | I386 | I387 | A395 | F413 | K417 | ARG | SER |
|------|------|------|------|------|------|------|-----|-----|

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 194518                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 35                                      | Depositor |
| Minimum defocus (nm)                 | 1250                                    | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.022                                   | Depositor |
| Minimum map value                    | -0.005                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.001                                   | Depositor |
| Recommended contour level            | 0.0016                                  | Depositor |
| Map size (Å)                         | 410.496, 410.496, 410.496               | wwPDB     |
| Map dimensions                       | 384, 384, 384                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.069, 1.069, 1.069                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$    |
| 1   | 8     | 0.56         | 0/1283      | 0.79        | 1/1954 (0.1%)  |
| 2   | a     | 0.15         | 0/3329      | 0.29        | 0/4483         |
| 2   | b     | 0.18         | 0/3329      | 0.33        | 0/4483         |
| 2   | c     | 0.20         | 0/3329      | 0.34        | 1/4483 (0.0%)  |
| 2   | d     | 0.18         | 0/3329      | 0.32        | 0/4483         |
| 2   | e     | 0.19         | 0/3329      | 0.35        | 1/4483 (0.0%)  |
| 2   | f     | 0.20         | 0/3329      | 0.35        | 1/4483 (0.0%)  |
| All | All   | 0.22         | 0/21257     | 0.38        | 4/28852 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | b     | 0                   | 1                   |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | 8     | 41  | DC   | O4'-C1'-N1 | 16.77 | 133.56      | 108.40   |
| 2   | f     | 322 | ASP  | N-CA-C     | -5.98 | 105.28      | 112.58   |
| 2   | e     | 334 | GLU  | N-CA-C     | -5.46 | 104.72      | 111.33   |
| 2   | c     | 334 | GLU  | N-CA-C     | -5.21 | 105.02      | 111.33   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | b     | 331 | ILE  | Mainchain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 8     | 1162  | 63       | 673      | 263     | 0            |
| 2   | a     | 3280  | 0        | 3357     | 231     | 0            |
| 2   | b     | 3280  | 0        | 3355     | 250     | 0            |
| 2   | c     | 3280  | 0        | 3354     | 279     | 0            |
| 2   | d     | 3280  | 0        | 3355     | 245     | 0            |
| 2   | e     | 3280  | 0        | 3352     | 282     | 0            |
| 2   | f     | 3280  | 0        | 3355     | 302     | 0            |
| 3   | a     | 27    | 0        | 12       | 58      | 0            |
| 3   | b     | 27    | 0        | 12       | 59      | 0            |
| 3   | c     | 27    | 0        | 12       | 53      | 0            |
| 3   | d     | 27    | 0        | 12       | 56      | 0            |
| 3   | e     | 27    | 0        | 12       | 56      | 0            |
| 3   | f     | 27    | 0        | 12       | 62      | 0            |
| 4   | a     | 1     | 0        | 0        | 0       | 0            |
| 4   | b     | 1     | 0        | 0        | 0       | 0            |
| 4   | c     | 1     | 0        | 0        | 0       | 0            |
| 4   | d     | 1     | 0        | 0        | 0       | 0            |
| 4   | e     | 1     | 0        | 0        | 0       | 0            |
| 4   | f     | 1     | 0        | 0        | 0       | 0            |
| 5   | a     | 4     | 0        | 0        | 3       | 0            |
| 5   | b     | 4     | 0        | 0        | 3       | 0            |
| 5   | c     | 4     | 0        | 0        | 3       | 0            |
| 5   | d     | 4     | 0        | 0        | 3       | 0            |
| 5   | e     | 4     | 0        | 0        | 3       | 0            |
| 5   | f     | 4     | 0        | 0        | 3       | 0            |
| All | All   | 21034 | 63       | 20873    | 1228    | 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 29.

All (1228) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:c:286:THR:CG2  | 2:b:326:LYS:HE3  | 1.23                     | 1.63              |
| 1:8:1:DC:C5      | 2:f:116:VAL:HG13 | 1.11                     | 1.63              |
| 2:e:286:THR:HG21 | 2:d:326:LYS:CE   | 1.11                     | 1.59              |
| 1:8:11:DC:C2'    | 2:a:88:ARG:HH11  | 1.12                     | 1.59              |
| 2:e:326:LYS:HE3  | 2:f:286:THR:CG2  | 1.23                     | 1.58              |
| 1:8:1:DC:C4      | 2:f:116:VAL:CG1  | 1.88                     | 1.56              |
| 2:c:286:THR:HG21 | 2:b:326:LYS:CE   | 1.14                     | 1.54              |
| 2:c:326:LYS:CE   | 2:d:286:THR:CG2  | 1.78                     | 1.54              |
| 2:e:286:THR:CG2  | 2:d:326:LYS:HE3  | 1.36                     | 1.53              |
| 2:c:286:THR:CG2  | 2:b:326:LYS:CE   | 1.78                     | 1.52              |
| 2:c:326:LYS:HE3  | 2:d:286:THR:CG2  | 1.25                     | 1.52              |
| 2:c:366:ARG:NH1  | 2:b:181:LYS:CA   | 1.68                     | 1.52              |
| 2:e:181:LYS:CA   | 2:f:366:ARG:NH1  | 1.70                     | 1.51              |
| 2:e:366:ARG:HH11 | 2:d:181:LYS:CA   | 1.22                     | 1.50              |
| 2:c:181:LYS:CA   | 2:d:366:ARG:NH1  | 1.77                     | 1.45              |
| 1:8:11:DC:H2'    | 2:a:88:ARG:NH1   | 1.19                     | 1.44              |
| 1:8:11:DC:C6     | 2:a:88:ARG:NH1   | 1.86                     | 1.43              |
| 2:e:286:THR:CG2  | 2:d:326:LYS:CE   | 1.91                     | 1.43              |
| 2:e:366:ARG:NH1  | 2:d:181:LYS:HA   | 1.14                     | 1.43              |
| 2:e:326:LYS:CE   | 2:f:286:THR:HG21 | 0.98                     | 1.42              |
| 2:c:326:LYS:CE   | 2:d:286:THR:HG21 | 0.95                     | 1.41              |
| 1:8:1:DC:C4      | 2:f:116:VAL:HG13 | 1.45                     | 1.41              |
| 2:b:138:PRO:HB2  | 2:a:214:GLU:CA   | 1.51                     | 1.41              |
| 2:c:181:LYS:CA   | 2:d:366:ARG:HH11 | 1.30                     | 1.41              |
| 2:c:181:LYS:HA   | 2:d:366:ARG:NH1  | 1.15                     | 1.40              |
| 2:f:214:GLU:CA   | 2:a:138:PRO:HB2  | 1.52                     | 1.40              |
| 2:e:366:ARG:NH1  | 2:d:181:LYS:CA   | 1.78                     | 1.40              |
| 2:e:326:LYS:CE   | 2:f:286:THR:CG2  | 1.80                     | 1.39              |
| 2:c:286:THR:CG2  | 2:b:326:LYS:NZ   | 1.87                     | 1.37              |
| 1:8:1:DC:N4      | 2:f:116:VAL:HG11 | 1.36                     | 1.37              |
| 2:e:181:LYS:HA   | 2:f:366:ARG:NH1  | 1.09                     | 1.35              |
| 2:c:286:THR:CB   | 2:b:326:LYS:CE   | 2.02                     | 1.35              |
| 2:e:214:GLU:CA   | 2:f:138:PRO:HB2  | 1.55                     | 1.35              |
| 1:8:1:DC:C5      | 2:f:116:VAL:CG1  | 2.05                     | 1.34              |
| 1:8:1:DC:P       | 2:f:115:LYS:CE   | 2.17                     | 1.33              |
| 1:8:57:DC:H2''   | 2:e:109:ARG:NH1  | 1.43                     | 1.32              |
| 2:c:138:PRO:HB2  | 2:b:214:GLU:CA   | 1.59                     | 1.31              |
| 2:f:186:MET:SD   | 2:a:367:LYS:NZ   | 2.01                     | 1.31              |
| 3:f:1000:ADP:C5' | 2:a:366:ARG:HD3  | 1.60                     | 1.30              |
| 2:c:366:ARG:HB3  | 3:b:1000:ADP:O3' | 1.17                     | 1.28              |
| 2:e:366:ARG:HB3  | 3:d:1000:ADP:O3' | 1.23                     | 1.27              |
| 2:c:366:ARG:NH1  | 2:b:181:LYS:HA   | 0.96                     | 1.27              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:b:385:LYS:NZ   | 2:a:352:LYS:O    | 1.64                     | 1.27              |
| 2:b:366:ARG:HB3  | 3:a:1000:ADP:O3' | 1.29                     | 1.25              |
| 2:e:367:LYS:NZ   | 2:d:186:MET:SD   | 2.09                     | 1.25              |
| 2:c:214:GLU:CA   | 2:d:138:PRO:HB2  | 1.65                     | 1.25              |
| 2:e:286:THR:CG2  | 2:d:326:LYS:NZ   | 2.00                     | 1.24              |
| 2:c:385:LYS:NZ   | 2:b:352:LYS:O    | 1.67                     | 1.24              |
| 1:8:57:DC:C2'    | 2:e:109:ARG:NH1  | 1.99                     | 1.24              |
| 2:f:184:LYS:HG3  | 3:f:1000:ADP:O3B | 1.38                     | 1.24              |
| 2:e:184:LYS:HB2  | 3:e:1000:ADP:O2B | 1.36                     | 1.24              |
| 2:d:184:LYS:HB2  | 3:d:1000:ADP:O3B | 1.36                     | 1.24              |
| 2:f:184:LYS:HB2  | 3:f:1000:ADP:O2B | 1.36                     | 1.24              |
| 2:b:184:LYS:HB2  | 3:b:1000:ADP:O1B | 1.36                     | 1.24              |
| 1:8:1:DC:C5'     | 2:f:115:LYS:HE3  | 1.68                     | 1.24              |
| 2:f:347:ARG:HH22 | 2:a:336:LYS:NZ   | 1.33                     | 1.23              |
| 2:d:184:LYS:HG3  | 3:d:1000:ADP:O1B | 1.38                     | 1.23              |
| 1:8:21:DC:C6     | 2:b:88:ARG:NH1   | 2.06                     | 1.23              |
| 2:a:184:LYS:HB2  | 3:a:1000:ADP:O1B | 1.36                     | 1.23              |
| 2:c:184:LYS:HB2  | 3:c:1000:ADP:O3B | 1.36                     | 1.23              |
| 2:c:367:LYS:NZ   | 2:b:186:MET:SD   | 2.09                     | 1.23              |
| 2:a:184:LYS:HG3  | 3:a:1000:ADP:O3B | 1.38                     | 1.23              |
| 3:e:1000:ADP:O3' | 2:f:366:ARG:HB3  | 1.32                     | 1.22              |
| 2:d:355:PHE:CE1  | 3:d:1000:ADP:C4  | 2.27                     | 1.22              |
| 2:f:272:ARG:NH1  | 2:a:334:GLU:OE2  | 1.70                     | 1.22              |
| 2:c:184:LYS:HG3  | 3:c:1000:ADP:O1B | 1.38                     | 1.22              |
| 1:8:1:DC:O5'     | 2:f:115:LYS:CE   | 1.86                     | 1.22              |
| 2:e:138:PRO:HB2  | 2:d:214:GLU:CA   | 1.70                     | 1.22              |
| 2:e:355:PHE:CE1  | 3:e:1000:ADP:C4  | 2.27                     | 1.22              |
| 2:a:355:PHE:CE1  | 3:a:1000:ADP:C4  | 2.27                     | 1.22              |
| 1:8:1:DC:C4      | 2:f:116:VAL:HG11 | 1.64                     | 1.21              |
| 2:c:355:PHE:CE1  | 3:c:1000:ADP:C4  | 2.27                     | 1.21              |
| 3:f:1000:ADP:O3' | 2:a:366:ARG:HB3  | 1.06                     | 1.21              |
| 1:8:53:DC:C4     | 2:e:85:GLN:NE2   | 2.09                     | 1.21              |
| 2:f:355:PHE:CE1  | 3:f:1000:ADP:C4  | 2.27                     | 1.21              |
| 2:b:355:PHE:CE1  | 3:b:1000:ADP:C4  | 2.27                     | 1.21              |
| 2:b:184:LYS:HG3  | 3:b:1000:ADP:O3B | 1.38                     | 1.20              |
| 2:c:138:PRO:HB2  | 2:b:214:GLU:HA   | 1.20                     | 1.19              |
| 2:e:186:MET:SD   | 2:f:367:LYS:NZ   | 2.17                     | 1.18              |
| 2:c:366:ARG:HD3  | 3:b:1000:ADP:C5' | 1.74                     | 1.18              |
| 1:8:53:DC:N4     | 2:e:85:GLN:NE2   | 1.92                     | 1.18              |
| 2:c:286:THR:CB   | 2:b:326:LYS:HZ1  | 1.57                     | 1.18              |
| 2:e:184:LYS:HG3  | 3:e:1000:ADP:O3B | 1.38                     | 1.17              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:e:181:LYS:N     | 2:f:366:ARG:NH1  | 1.91                     | 1.17              |
| 2:f:347:ARG:NH2   | 2:a:336:LYS:NZ   | 1.92                     | 1.17              |
| 3:c:1000:ADP:H5'2 | 2:d:366:ARG:HD3  | 1.25                     | 1.17              |
| 2:c:138:PRO:CG    | 2:b:213:PRO:HB2  | 1.75                     | 1.16              |
| 1:8:40:DC:O5'     | 2:d:87:ARG:NH1   | 1.77                     | 1.16              |
| 2:b:366:ARG:HD3   | 3:a:1000:ADP:C5' | 1.74                     | 1.16              |
| 1:8:2:DC:H41      | 2:f:115:LYS:CA   | 1.58                     | 1.16              |
| 1:8:1:DC:H41      | 2:f:116:VAL:CG2  | 1.58                     | 1.15              |
| 1:8:33:DC:H41     | 2:c:85:GLN:NE2   | 1.42                     | 1.14              |
| 2:f:272:ARG:HH12  | 2:a:334:GLU:CD   | 1.55                     | 1.14              |
| 2:c:286:THR:HB    | 2:b:326:LYS:NZ   | 1.63                     | 1.14              |
| 1:8:57:DC:C2'     | 2:e:109:ARG:HH12 | 1.60                     | 1.14              |
| 2:e:326:LYS:NZ    | 2:f:286:THR:CG2  | 2.10                     | 1.14              |
| 2:f:214:GLU:HA    | 2:a:138:PRO:HB2  | 1.16                     | 1.13              |
| 3:f:1000:ADP:H4'  | 2:a:366:ARG:HG2  | 1.27                     | 1.13              |
| 1:8:40:DC:O5'     | 2:d:87:ARG:CZ    | 1.96                     | 1.12              |
| 3:e:1000:ADP:C5'  | 2:f:366:ARG:HD3  | 1.77                     | 1.13              |
| 2:c:214:GLU:HA    | 2:d:138:PRO:HB2  | 1.22                     | 1.12              |
| 2:f:352:LYS:O     | 2:a:385:LYS:NZ   | 1.81                     | 1.12              |
| 1:8:1:DC:H41      | 2:f:116:VAL:HG21 | 1.08                     | 1.12              |
| 2:b:336:LYS:NZ    | 2:a:347:ARG:HH22 | 1.46                     | 1.12              |
| 2:e:352:LYS:HG2   | 2:f:385:LYS:NZ   | 1.63                     | 1.12              |
| 2:e:366:ARG:HD3   | 3:d:1000:ADP:C5' | 1.79                     | 1.11              |
| 2:c:138:PRO:HG2   | 2:b:213:PRO:HB2  | 1.26                     | 1.11              |
| 2:e:138:PRO:HB2   | 2:d:214:GLU:HA   | 1.32                     | 1.11              |
| 2:e:214:GLU:HA    | 2:f:138:PRO:HB2  | 1.13                     | 1.11              |
| 2:e:138:PRO:HG2   | 2:d:213:PRO:HB2  | 1.21                     | 1.11              |
| 2:b:305:ARG:NH2   | 2:a:213:PRO:HG2  | 1.63                     | 1.11              |
| 2:c:286:THR:CB    | 2:b:326:LYS:NZ   | 2.08                     | 1.11              |
| 1:8:11:DC:C1'     | 2:a:88:ARG:HG3   | 1.80                     | 1.10              |
| 1:8:21:DC:C1'     | 2:b:88:ARG:HG3   | 1.81                     | 1.10              |
| 2:e:138:PRO:CG    | 2:d:213:PRO:HB2  | 1.79                     | 1.10              |
| 2:b:367:LYS:NZ    | 2:a:186:MET:SD   | 2.23                     | 1.10              |
| 1:8:1:DC:C5'      | 2:f:115:LYS:HG3  | 1.80                     | 1.10              |
| 2:e:366:ARG:NH1   | 2:d:181:LYS:N    | 1.98                     | 1.10              |
| 2:b:138:PRO:HB2   | 2:a:214:GLU:HA   | 1.12                     | 1.09              |
| 2:b:138:PRO:HG2   | 2:a:213:PRO:C    | 1.76                     | 1.09              |
| 2:e:181:LYS:HA    | 2:f:366:ARG:CZ   | 1.82                     | 1.09              |
| 2:e:324:GLY:HA3   | 2:f:333:GLU:HB3  | 1.17                     | 1.09              |
| 3:f:1000:ADP:O3'  | 2:a:366:ARG:CB   | 1.99                     | 1.09              |
| 3:c:1000:ADP:O3'  | 2:d:366:ARG:HB3  | 1.50                     | 1.09              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:c:352:LYS:HG2   | 2:d:385:LYS:NZ   | 1.67                     | 1.09              |
| 2:f:347:ARG:NH2   | 2:a:336:LYS:HZ1  | 1.49                     | 1.09              |
| 2:f:184:LYS:NZ    | 5:f:1002:BEF:F2  | 1.76                     | 1.08              |
| 2:c:181:LYS:N     | 2:d:366:ARG:NH1  | 1.99                     | 1.08              |
| 2:c:326:LYS:HZ1   | 2:d:286:THR:HG22 | 1.15                     | 1.08              |
| 2:c:185:THR:N     | 3:c:1000:ADP:O1A | 1.86                     | 1.08              |
| 2:c:184:LYS:NZ    | 5:c:1002:BEF:F2  | 1.76                     | 1.08              |
| 2:b:138:PRO:CG    | 2:a:213:PRO:HB2  | 1.82                     | 1.08              |
| 1:8:1:DC:P        | 2:f:115:LYS:HE3  | 1.89                     | 1.08              |
| 2:d:184:LYS:NZ    | 5:d:1002:BEF:F2  | 1.76                     | 1.08              |
| 1:8:1:DC:N4       | 2:f:116:VAL:CG1  | 2.00                     | 1.07              |
| 2:b:185:THR:N     | 3:b:1000:ADP:O1A | 1.86                     | 1.07              |
| 2:a:184:LYS:NZ    | 5:a:1002:BEF:F2  | 1.76                     | 1.07              |
| 1:8:1:DC:O5'      | 2:f:115:LYS:HE2  | 1.47                     | 1.07              |
| 2:b:184:LYS:NZ    | 5:b:1002:BEF:F2  | 1.76                     | 1.07              |
| 2:e:184:LYS:NZ    | 5:e:1002:BEF:F2  | 1.76                     | 1.07              |
| 2:e:185:THR:N     | 3:e:1000:ADP:O2A | 1.86                     | 1.07              |
| 1:8:53:DC:C5      | 2:e:85:GLN:NE2   | 2.23                     | 1.07              |
| 2:d:185:THR:N     | 3:d:1000:ADP:O2A | 1.87                     | 1.07              |
| 1:8:21:DC:C2      | 2:b:88:ARG:HG3   | 1.90                     | 1.06              |
| 2:c:138:PRO:HG2   | 2:b:213:PRO:CB   | 1.85                     | 1.06              |
| 2:c:326:LYS:HE2   | 2:d:286:THR:HG21 | 1.35                     | 1.06              |
| 2:b:355:PHE:CD1   | 3:b:1000:ADP:C5  | 2.44                     | 1.06              |
| 2:a:185:THR:N     | 3:a:1000:ADP:O1A | 1.86                     | 1.06              |
| 2:f:185:THR:N     | 3:f:1000:ADP:O2A | 1.86                     | 1.06              |
| 2:c:366:ARG:NH1   | 2:b:181:LYS:N    | 2.04                     | 1.06              |
| 2:c:326:LYS:NZ    | 2:d:286:THR:CG2  | 2.17                     | 1.06              |
| 2:a:355:PHE:CD1   | 3:a:1000:ADP:C5  | 2.43                     | 1.06              |
| 2:d:355:PHE:CD1   | 3:d:1000:ADP:C5  | 2.43                     | 1.06              |
| 1:8:54:DC:H5''    | 1:8:54:DC:H6     | 1.20                     | 1.06              |
| 3:f:1000:ADP:C5'  | 2:a:366:ARG:CD   | 2.34                     | 1.06              |
| 2:c:355:PHE:CD1   | 3:c:1000:ADP:C5  | 2.43                     | 1.06              |
| 1:8:34:DC:O2      | 2:c:80:TYR:OH    | 1.71                     | 1.05              |
| 3:f:1000:ADP:H5'2 | 2:a:366:ARG:CD   | 1.84                     | 1.05              |
| 1:8:53:DC:N4      | 2:e:85:GLN:HE22  | 1.50                     | 1.05              |
| 2:f:355:PHE:CD1   | 3:f:1000:ADP:C5  | 2.44                     | 1.05              |
| 2:b:385:LYS:HZ2   | 2:a:352:LYS:HG2  | 1.17                     | 1.05              |
| 2:e:138:PRO:HG2   | 2:d:213:PRO:CB   | 1.87                     | 1.05              |
| 2:e:286:THR:CG2   | 2:d:326:LYS:HZ1  | 1.62                     | 1.05              |
| 2:c:333:GLU:HB3   | 2:b:324:GLY:HA3  | 1.33                     | 1.05              |
| 1:8:7:DC:H2''     | 2:f:109:ARG:HH12 | 1.19                     | 1.05              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:e:355:PHE:CD1   | 3:e:1000:ADP:C5   | 2.43                     | 1.05              |
| 1:8:4:DC:H5''     | 1:8:4:DC:H6       | 1.20                     | 1.04              |
| 2:c:336:LYS:NZ    | 2:b:347:ARG:HH22  | 1.53                     | 1.04              |
| 2:c:366:ARG:CZ    | 2:b:181:LYS:HA    | 1.86                     | 1.04              |
| 1:8:2:DC:H41      | 2:f:115:LYS:N     | 1.56                     | 1.04              |
| 1:8:13:DC:N4      | 2:a:114:LEU:HD13  | 1.71                     | 1.04              |
| 2:f:218:GLU:CD    | 2:a:140:HIS:HE2   | 1.66                     | 1.03              |
| 1:8:7:DC:C2'      | 2:f:109:ARG:HH12  | 1.70                     | 1.03              |
| 2:e:286:THR:CB    | 2:d:326:LYS:CE    | 2.37                     | 1.03              |
| 3:e:1000:ADP:H5'2 | 2:f:366:ARG:HD3   | 1.08                     | 1.03              |
| 2:b:138:PRO:HG2   | 2:a:213:PRO:HB2   | 1.39                     | 1.03              |
| 2:b:366:ARG:HD3   | 3:a:1000:ADP:H5'2 | 1.08                     | 1.03              |
| 1:8:1:DC:H5'      | 2:f:115:LYS:HG3   | 1.39                     | 1.02              |
| 2:c:181:LYS:HA    | 2:d:366:ARG:CZ    | 1.89                     | 1.02              |
| 2:c:366:ARG:HD3   | 3:b:1000:ADP:H5'2 | 1.04                     | 1.02              |
| 1:8:1:DC:C5'      | 2:f:115:LYS:CE    | 2.36                     | 1.02              |
| 1:8:2:DC:N4       | 2:f:115:LYS:CA    | 2.21                     | 1.02              |
| 1:8:33:DC:N4      | 2:c:85:GLN:CD     | 2.17                     | 1.02              |
| 1:8:44:DC:H5''    | 1:8:44:DC:H6      | 1.20                     | 1.01              |
| 2:c:366:ARG:HG2   | 3:b:1000:ADP:H4'  | 1.40                     | 1.01              |
| 2:f:213:PRO:HB2   | 2:a:138:PRO:HG2   | 1.41                     | 1.01              |
| 2:c:366:ARG:CB    | 3:b:1000:ADP:O3'  | 2.08                     | 1.01              |
| 1:8:13:DC:H41     | 2:a:114:LEU:HD13  | 0.89                     | 1.01              |
| 2:c:138:PRO:HG2   | 2:b:213:PRO:C     | 1.85                     | 1.01              |
| 1:8:1:DC:P        | 2:f:115:LYS:HE2   | 1.90                     | 1.01              |
| 1:8:11:DC:N1      | 2:a:88:ARG:NH1    | 2.09                     | 1.01              |
| 2:c:286:THR:CG2   | 2:b:326:LYS:HZ1   | 1.62                     | 1.01              |
| 2:b:336:LYS:HZ1   | 2:a:347:ARG:NH2   | 1.57                     | 1.01              |
| 2:d:355:PHE:CE1   | 3:d:1000:ADP:N9   | 2.29                     | 1.01              |
| 2:e:355:PHE:CE1   | 3:e:1000:ADP:N9   | 2.29                     | 1.00              |
| 2:e:333:GLU:HB3   | 2:d:324:GLY:HA3   | 1.43                     | 1.00              |
| 2:e:366:ARG:HD3   | 3:d:1000:ADP:H5'2 | 1.04                     | 1.00              |
| 1:8:13:DC:H41     | 2:a:114:LEU:CD1   | 1.75                     | 0.99              |
| 2:c:140:HIS:HE2   | 2:b:218:GLU:CD    | 1.69                     | 0.99              |
| 1:8:21:DC:H1'     | 2:b:88:ARG:HG3    | 1.41                     | 0.99              |
| 2:b:355:PHE:CE1   | 3:b:1000:ADP:N9   | 2.29                     | 0.99              |
| 2:e:324:GLY:HA3   | 2:f:333:GLU:CB    | 1.91                     | 0.99              |
| 2:c:366:ARG:HH12  | 2:b:181:LYS:N     | 1.60                     | 0.99              |
| 2:e:366:ARG:CZ    | 2:d:181:LYS:HA    | 1.92                     | 0.99              |
| 2:a:355:PHE:CE1   | 3:a:1000:ADP:N9   | 2.29                     | 0.99              |
| 2:f:355:PHE:CE1   | 3:f:1000:ADP:N9   | 2.29                     | 0.99              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:c:355:PHE:CE1  | 3:c:1000:ADP:N9   | 2.29                     | 0.99              |
| 2:e:286:THR:HG21 | 2:d:326:LYS:NZ    | 1.71                     | 0.99              |
| 2:e:366:ARG:HH12 | 2:d:181:LYS:H     | 0.99                     | 0.98              |
| 2:c:366:ARG:CD   | 3:b:1000:ADP:H5'2 | 1.93                     | 0.98              |
| 2:b:305:ARG:CZ   | 2:a:213:PRO:HG2   | 1.93                     | 0.98              |
| 1:8:1:DC:H5'     | 2:f:115:LYS:HE3   | 1.42                     | 0.98              |
| 2:e:347:ARG:HH22 | 2:f:336:LYS:NZ    | 1.62                     | 0.98              |
| 2:e:366:ARG:HG2  | 3:d:1000:ADP:H4'  | 1.42                     | 0.98              |
| 1:8:11:DC:H6     | 2:a:88:ARG:HH12   | 0.99                     | 0.97              |
| 2:e:366:ARG:CB   | 3:d:1000:ADP:O3'  | 2.12                     | 0.97              |
| 2:c:336:LYS:HZ3  | 2:b:347:ARG:HH22  | 1.10                     | 0.97              |
| 3:c:1000:ADP:C5' | 2:d:366:ARG:HD3   | 1.93                     | 0.97              |
| 1:8:33:DC:H41    | 2:c:85:GLN:CD     | 1.70                     | 0.97              |
| 2:c:305:ARG:NH2  | 2:b:213:PRO:HG2   | 1.80                     | 0.97              |
| 2:c:181:LYS:CB   | 2:d:366:ARG:HH11  | 1.77                     | 0.96              |
| 2:e:181:LYS:N    | 2:f:366:ARG:HH12  | 1.55                     | 0.96              |
| 3:f:1000:ADP:H4' | 2:a:366:ARG:CG    | 1.94                     | 0.96              |
| 1:8:1:DC:C5'     | 2:f:115:LYS:CG    | 2.43                     | 0.96              |
| 2:c:336:LYS:NZ   | 2:b:347:ARG:NH2   | 2.12                     | 0.96              |
| 1:8:11:DC:C1'    | 2:a:88:ARG:HH11   | 1.78                     | 0.96              |
| 2:b:385:LYS:NZ   | 2:a:352:LYS:HG2   | 1.79                     | 0.96              |
| 2:e:183:GLY:C    | 3:e:1000:ADP:O2A  | 2.09                     | 0.95              |
| 2:c:183:GLY:C    | 3:c:1000:ADP:O1A  | 2.09                     | 0.95              |
| 2:f:183:GLY:C    | 3:f:1000:ADP:O2A  | 2.09                     | 0.95              |
| 2:b:138:PRO:HG2  | 2:a:213:PRO:CB    | 1.95                     | 0.95              |
| 2:d:183:GLY:C    | 3:d:1000:ADP:O2A  | 2.09                     | 0.95              |
| 1:8:2:DC:C5      | 2:f:115:LYS:HA    | 2.01                     | 0.95              |
| 2:e:366:ARG:CD   | 3:d:1000:ADP:H5'2 | 1.94                     | 0.95              |
| 2:c:286:THR:HG22 | 2:b:326:LYS:NZ    | 1.81                     | 0.95              |
| 2:b:336:LYS:NZ   | 2:a:347:ARG:NH2   | 2.13                     | 0.95              |
| 1:8:11:DC:H1'    | 2:a:88:ARG:CG     | 1.95                     | 0.95              |
| 1:8:11:DC:H1'    | 2:a:88:ARG:HG3    | 0.98                     | 0.95              |
| 1:8:41:DC:H1'    | 2:d:88:ARG:NH1    | 1.79                     | 0.95              |
| 2:e:326:LYS:CE   | 2:f:286:THR:CB    | 2.43                     | 0.95              |
| 2:c:286:THR:CB   | 2:b:326:LYS:HE2   | 1.96                     | 0.95              |
| 2:a:183:GLY:C    | 3:a:1000:ADP:O1A  | 2.09                     | 0.95              |
| 1:8:2:DC:C4      | 2:f:115:LYS:HA    | 2.02                     | 0.95              |
| 2:c:140:HIS:NE2  | 2:b:218:GLU:OE2   | 1.99                     | 0.95              |
| 2:c:366:ARG:HH12 | 2:b:181:LYS:H     | 1.05                     | 0.95              |
| 1:8:2:DC:O2      | 2:f:89:PHE:HE2    | 1.49                     | 0.94              |
| 2:e:326:LYS:HZ1  | 2:f:286:THR:CG2   | 1.77                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:e:213:PRO:HB2   | 2:f:138:PRO:HG2   | 1.45                     | 0.94              |
| 2:c:186:MET:SD    | 2:d:367:LYS:NZ    | 2.40                     | 0.94              |
| 2:b:183:GLY:C     | 3:b:1000:ADP:O1A  | 2.09                     | 0.94              |
| 2:e:326:LYS:NZ    | 2:f:286:THR:HG22  | 1.83                     | 0.94              |
| 2:e:218:GLU:CD    | 2:f:140:HIS:HE2   | 1.75                     | 0.94              |
| 2:e:366:ARG:HB3   | 3:d:1000:ADP:HO3' | 0.98                     | 0.94              |
| 2:c:181:LYS:H     | 2:d:366:ARG:HH12  | 0.99                     | 0.94              |
| 2:c:286:THR:HB    | 2:b:326:LYS:HZ1   | 1.21                     | 0.94              |
| 2:a:184:LYS:CG    | 3:a:1000:ADP:O3B  | 2.16                     | 0.94              |
| 2:e:140:HIS:HE2   | 2:d:218:GLU:CD    | 1.75                     | 0.94              |
| 2:e:140:HIS:NE2   | 2:d:218:GLU:OE2   | 2.01                     | 0.94              |
| 2:f:218:GLU:OE2   | 2:a:140:HIS:NE2   | 2.00                     | 0.94              |
| 2:c:355:PHE:CD1   | 3:c:1000:ADP:C4   | 2.56                     | 0.94              |
| 2:b:355:PHE:CD1   | 3:b:1000:ADP:C4   | 2.56                     | 0.93              |
| 2:a:355:PHE:CD1   | 3:a:1000:ADP:C4   | 2.56                     | 0.93              |
| 3:f:1000:ADP:H5'2 | 2:a:366:ARG:HD3   | 0.94                     | 0.93              |
| 1:8:57:DC:H2''    | 2:e:109:ARG:HH12  | 1.06                     | 0.93              |
| 1:8:57:DC:H2''    | 2:e:109:ARG:CZ    | 1.98                     | 0.93              |
| 2:f:184:LYS:CG    | 3:f:1000:ADP:O3B  | 2.16                     | 0.93              |
| 2:d:184:LYS:CG    | 3:d:1000:ADP:O1B  | 2.16                     | 0.93              |
| 1:8:3:DC:H3'      | 1:8:3:DC:O2       | 1.68                     | 0.93              |
| 2:f:355:PHE:CD1   | 3:f:1000:ADP:C4   | 2.56                     | 0.93              |
| 2:e:181:LYS:H     | 2:f:366:ARG:NH1   | 1.59                     | 0.93              |
| 1:8:1:DC:H5'      | 2:f:115:LYS:CG    | 1.99                     | 0.93              |
| 2:c:280:ALA:CB    | 2:d:283:LYS:HD3   | 1.97                     | 0.93              |
| 2:b:366:ARG:HG2   | 3:a:1000:ADP:H4'  | 1.51                     | 0.93              |
| 1:8:21:DC:N1      | 2:b:88:ARG:HG3    | 1.84                     | 0.92              |
| 3:f:1000:ADP:HO3' | 2:a:366:ARG:HB3   | 1.14                     | 0.92              |
| 2:e:184:LYS:CG    | 3:e:1000:ADP:O3B  | 2.16                     | 0.92              |
| 2:f:347:ARG:HH22  | 2:a:336:LYS:HZ3   | 0.94                     | 0.92              |
| 2:b:138:PRO:HB2   | 2:a:214:GLU:N     | 1.83                     | 0.92              |
| 2:c:366:ARG:CD    | 3:b:1000:ADP:C5'  | 2.47                     | 0.92              |
| 2:b:140:HIS:HE2   | 2:a:218:GLU:CD    | 1.78                     | 0.92              |
| 1:8:11:DC:C1'     | 2:a:88:ARG:NH1    | 2.32                     | 0.92              |
| 2:b:366:ARG:HB3   | 3:a:1000:ADP:HO3' | 1.34                     | 0.92              |
| 2:d:355:PHE:CD1   | 3:d:1000:ADP:C4   | 2.56                     | 0.92              |
| 2:c:138:PRO:HB2   | 2:b:214:GLU:N     | 1.82                     | 0.92              |
| 2:b:184:LYS:CG    | 3:b:1000:ADP:O3B  | 2.16                     | 0.92              |
| 2:c:184:LYS:CG    | 3:c:1000:ADP:O1B  | 2.16                     | 0.92              |
| 1:8:11:DC:C2'     | 2:a:88:ARG:NH1    | 1.89                     | 0.92              |
| 2:d:333:GLU:C     | 2:d:335:PHE:H     | 1.77                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:b:285:LEU:HG    | 2:a:288:GLY:HA3   | 1.51                     | 0.92              |
| 2:e:355:PHE:CD1   | 3:e:1000:ADP:C4   | 2.56                     | 0.91              |
| 2:c:326:LYS:NZ    | 2:d:286:THR:HG22  | 1.82                     | 0.91              |
| 2:f:214:GLU:CA    | 2:a:138:PRO:CB    | 2.46                     | 0.91              |
| 2:b:366:ARG:CD    | 3:a:1000:ADP:H5'2 | 1.99                     | 0.91              |
| 2:c:286:THR:HB    | 2:b:326:LYS:CE    | 1.96                     | 0.90              |
| 1:8:1:DC:N3       | 2:f:89:PHE:CD1    | 2.19                     | 0.90              |
| 1:8:2:DC:N4       | 2:f:115:LYS:HA    | 1.85                     | 0.90              |
| 2:f:214:GLU:N     | 2:a:138:PRO:HB2   | 1.84                     | 0.90              |
| 2:f:272:ARG:CZ    | 2:a:334:GLU:OE2   | 2.19                     | 0.90              |
| 2:e:326:LYS:HZ1   | 2:f:286:THR:HG22  | 1.32                     | 0.90              |
| 2:e:366:ARG:HH11  | 2:d:181:LYS:CB    | 1.85                     | 0.90              |
| 2:c:286:THR:CB    | 2:b:326:LYS:HE3   | 1.86                     | 0.90              |
| 2:b:366:ARG:CD    | 3:a:1000:ADP:C5'  | 2.50                     | 0.90              |
| 3:e:1000:ADP:HO3' | 2:f:366:ARG:HB3   | 1.35                     | 0.90              |
| 2:f:184:LYS:N     | 3:f:1000:ADP:O2A  | 2.05                     | 0.90              |
| 2:c:181:LYS:N     | 2:d:366:ARG:HH12  | 1.61                     | 0.89              |
| 1:8:1:DC:H5'      | 2:f:115:LYS:CE    | 2.02                     | 0.89              |
| 3:e:1000:ADP:H4'  | 2:f:366:ARG:HG2   | 1.54                     | 0.89              |
| 2:e:214:GLU:N     | 2:f:138:PRO:HB2   | 1.85                     | 0.89              |
| 2:e:366:ARG:HH12  | 2:d:181:LYS:N     | 1.64                     | 0.89              |
| 2:e:366:ARG:CD    | 3:d:1000:ADP:C5'  | 2.51                     | 0.89              |
| 2:b:138:PRO:CB    | 2:a:214:GLU:CA    | 2.45                     | 0.89              |
| 2:e:286:THR:CB    | 2:d:326:LYS:HZ1   | 1.84                     | 0.89              |
| 2:d:184:LYS:N     | 3:d:1000:ADP:O2A  | 2.06                     | 0.89              |
| 2:e:184:LYS:N     | 3:e:1000:ADP:O2A  | 2.05                     | 0.89              |
| 1:8:8:DC:H2'      | 1:8:8:DC:O2       | 1.72                     | 0.89              |
| 2:e:214:GLU:CA    | 2:f:138:PRO:CB    | 2.49                     | 0.89              |
| 2:e:286:THR:HG22  | 2:d:326:LYS:HZ1   | 1.36                     | 0.89              |
| 2:f:181:LYS:HD2   | 2:a:342:GLU:OE1   | 1.71                     | 0.89              |
| 2:c:336:LYS:HZ1   | 2:b:347:ARG:NH2   | 1.70                     | 0.89              |
| 2:b:184:LYS:N     | 3:b:1000:ADP:O1A  | 2.06                     | 0.89              |
| 2:a:184:LYS:N     | 3:a:1000:ADP:O1A  | 2.06                     | 0.89              |
| 2:c:184:LYS:N     | 3:c:1000:ADP:O1A  | 2.06                     | 0.88              |
| 2:b:138:PRO:HG3   | 2:a:213:PRO:HB2   | 1.55                     | 0.88              |
| 1:8:54:DC:H5''    | 1:8:54:DC:C6      | 2.08                     | 0.88              |
| 2:e:181:LYS:H     | 2:f:366:ARG:HH12  | 0.92                     | 0.88              |
| 2:e:218:GLU:OE2   | 2:f:140:HIS:NE2   | 2.06                     | 0.88              |
| 2:f:324:GLY:HA3   | 2:a:333:GLU:HG3   | 1.53                     | 0.88              |
| 1:8:1:DC:H5       | 2:f:116:VAL:HG13  | 1.36                     | 0.88              |
| 3:e:1000:ADP:H5'2 | 2:f:366:ARG:CD    | 2.01                     | 0.88              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:c:366:ARG:HB3  | 3:b:1000:ADP:HO3' | 1.29                     | 0.88              |
| 2:c:385:LYS:HZ2  | 2:b:352:LYS:HG2   | 1.36                     | 0.88              |
| 1:8:18:DC:H2'    | 1:8:18:DC:O2      | 1.72                     | 0.88              |
| 2:e:280:ALA:CB   | 2:f:283:LYS:HD3   | 2.03                     | 0.88              |
| 2:c:138:PRO:HG3  | 2:b:213:PRO:HB2   | 1.56                     | 0.88              |
| 1:8:11:DC:C6     | 2:a:88:ARG:CZ     | 2.57                     | 0.87              |
| 1:8:44:DC:H5''   | 1:8:44:DC:C6      | 2.08                     | 0.87              |
| 2:e:347:ARG:HH22 | 2:f:336:LYS:HZ3   | 1.23                     | 0.87              |
| 2:f:183:GLY:HA2  | 3:f:1000:ADP:H8   | 1.39                     | 0.87              |
| 2:e:183:GLY:HA2  | 3:e:1000:ADP:O5'  | 1.75                     | 0.87              |
| 2:f:183:GLY:HA2  | 3:f:1000:ADP:O5'  | 1.74                     | 0.87              |
| 2:b:183:GLY:HA2  | 3:b:1000:ADP:H8   | 1.39                     | 0.87              |
| 2:c:183:GLY:HA2  | 3:c:1000:ADP:H8   | 1.39                     | 0.87              |
| 2:e:183:GLY:HA2  | 3:e:1000:ADP:H8   | 1.39                     | 0.87              |
| 2:e:385:LYS:NZ   | 2:d:352:LYS:HG2   | 1.89                     | 0.87              |
| 2:f:352:LYS:HG2  | 2:a:385:LYS:HZ2   | 1.39                     | 0.87              |
| 1:8:21:DC:C2     | 2:b:88:ARG:CG     | 2.57                     | 0.86              |
| 2:c:183:GLY:HA2  | 3:c:1000:ADP:O5'  | 1.75                     | 0.86              |
| 1:8:18:DC:O2     | 1:8:18:DC:C2'     | 2.23                     | 0.86              |
| 2:b:183:GLY:HA2  | 3:b:1000:ADP:O5'  | 1.74                     | 0.86              |
| 2:d:183:GLY:HA2  | 3:d:1000:ADP:H8   | 1.39                     | 0.86              |
| 1:8:8:DC:O2      | 1:8:8:DC:C2'      | 2.23                     | 0.86              |
| 2:a:183:GLY:HA2  | 3:a:1000:ADP:H8   | 1.39                     | 0.86              |
| 2:a:183:GLY:HA2  | 3:a:1000:ADP:O5'  | 1.74                     | 0.86              |
| 2:e:138:PRO:HB2  | 2:d:214:GLU:N     | 1.90                     | 0.86              |
| 2:c:326:LYS:HE2  | 2:d:286:THR:CG2   | 1.98                     | 0.86              |
| 2:e:138:PRO:HG2  | 2:d:213:PRO:C     | 2.00                     | 0.86              |
| 1:8:1:DC:N4      | 2:f:116:VAL:HG21  | 1.90                     | 0.85              |
| 2:d:183:GLY:HA2  | 3:d:1000:ADP:O5'  | 1.74                     | 0.85              |
| 2:f:184:LYS:CB   | 3:f:1000:ADP:O2B  | 2.24                     | 0.85              |
| 1:8:4:DC:H5''    | 1:8:4:DC:C6       | 2.08                     | 0.85              |
| 1:8:48:DT:O2     | 1:8:48:DT:C2'     | 2.23                     | 0.85              |
| 2:e:305:ARG:NH2  | 2:d:213:PRO:HG2   | 1.91                     | 0.85              |
| 1:8:1:DC:H5''    | 2:f:115:LYS:HG3   | 1.57                     | 0.85              |
| 1:8:48:DT:O2     | 1:8:48:DT:H2'     | 1.74                     | 0.85              |
| 2:c:286:THR:HG21 | 2:b:326:LYS:CD    | 2.07                     | 0.85              |
| 1:8:1:DC:C5      | 2:f:116:VAL:O     | 2.30                     | 0.85              |
| 1:8:1:DC:O5'     | 2:f:115:LYS:HE3   | 1.56                     | 0.85              |
| 1:8:34:DC:N3     | 2:c:80:TYR:CE2    | 2.44                     | 0.85              |
| 2:e:366:ARG:NH1  | 2:d:181:LYS:H     | 1.64                     | 0.85              |
| 2:f:214:GLU:CB   | 2:a:138:PRO:HB2   | 2.06                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:8:21:DC:C5     | 2:b:88:ARG:NH1   | 2.45                     | 0.85              |
| 1:8:28:DC:H2'    | 1:8:28:DC:O2     | 1.75                     | 0.85              |
| 2:b:138:PRO:CB   | 2:a:214:GLU:N    | 2.40                     | 0.85              |
| 2:c:181:LYS:H    | 2:d:366:ARG:NH1  | 1.67                     | 0.84              |
| 2:b:184:LYS:CB   | 3:b:1000:ADP:O1B | 2.24                     | 0.84              |
| 1:8:28:DC:O2     | 1:8:28:DC:C2'    | 2.23                     | 0.84              |
| 2:c:326:LYS:CE   | 2:d:286:THR:CB   | 2.54                     | 0.84              |
| 2:e:324:GLY:CA   | 2:f:333:GLU:HB3  | 2.05                     | 0.84              |
| 2:c:347:ARG:HH22 | 2:d:336:LYS:NZ   | 1.75                     | 0.84              |
| 1:8:57:DC:C3'    | 2:e:109:ARG:HH12 | 1.90                     | 0.84              |
| 2:c:305:ARG:CZ   | 2:b:213:PRO:HG2  | 2.07                     | 0.83              |
| 2:c:232:PHE:CZ   | 2:d:302:GLY:HA3  | 2.13                     | 0.83              |
| 1:8:40:DC:O4'    | 2:d:87:ARG:NE    | 2.04                     | 0.83              |
| 3:e:1000:ADP:C5' | 2:f:366:ARG:CD   | 2.54                     | 0.83              |
| 2:b:336:LYS:HZ3  | 2:a:347:ARG:HH22 | 1.23                     | 0.83              |
| 1:8:3:DC:H42     | 2:f:114:LEU:HD13 | 1.43                     | 0.83              |
| 1:8:33:DC:N4     | 2:c:85:GLN:HG3   | 1.92                     | 0.83              |
| 2:a:184:LYS:CB   | 3:a:1000:ADP:O1B | 2.24                     | 0.83              |
| 1:8:21:DC:O2     | 2:b:88:ARG:CG    | 2.26                     | 0.83              |
| 2:c:214:GLU:N    | 2:d:138:PRO:HB2  | 1.93                     | 0.83              |
| 2:c:213:PRO:HB2  | 2:d:138:PRO:HG2  | 1.60                     | 0.83              |
| 1:8:1:DC:OP1     | 2:f:115:LYS:HE3  | 1.77                     | 0.82              |
| 2:e:333:GLU:HG2  | 2:e:336:LYS:HD2  | 1.59                     | 0.82              |
| 3:e:1000:ADP:O3' | 2:f:366:ARG:CB   | 2.24                     | 0.82              |
| 2:c:286:THR:OG1  | 2:b:326:LYS:HE2  | 1.79                     | 0.82              |
| 2:f:214:GLU:N    | 2:a:138:PRO:CB   | 2.42                     | 0.82              |
| 2:e:184:LYS:CB   | 3:e:1000:ADP:O2B | 2.24                     | 0.82              |
| 2:e:333:GLU:CB   | 2:d:324:GLY:HA3  | 2.10                     | 0.82              |
| 1:8:33:DC:N4     | 2:c:85:GLN:CG    | 2.43                     | 0.82              |
| 1:8:1:DC:N4      | 2:f:116:VAL:CG2  | 2.41                     | 0.82              |
| 2:c:366:ARG:CG   | 3:b:1000:ADP:H4' | 2.10                     | 0.82              |
| 2:b:140:HIS:NE2  | 2:a:218:GLU:OE2  | 2.12                     | 0.82              |
| 2:b:333:GLU:HA   | 2:b:336:LYS:HB2  | 1.60                     | 0.82              |
| 1:8:40:DC:O2     | 2:d:87:ARG:O     | 1.97                     | 0.81              |
| 2:b:366:ARG:CB   | 3:a:1000:ADP:O3' | 2.23                     | 0.81              |
| 1:8:17:DC:H2''   | 2:a:109:ARG:HH12 | 1.44                     | 0.81              |
| 2:f:213:PRO:HB2  | 2:a:138:PRO:CG   | 2.11                     | 0.81              |
| 2:d:184:LYS:CB   | 3:d:1000:ADP:O3B | 2.24                     | 0.81              |
| 2:e:214:GLU:N    | 2:f:138:PRO:CB   | 2.44                     | 0.81              |
| 2:e:183:GLY:CA   | 3:e:1000:ADP:H8  | 1.94                     | 0.81              |
| 2:b:138:PRO:HB2  | 2:a:214:GLU:CB   | 2.11                     | 0.81              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:c:138:PRO:CB    | 2:b:214:GLU:N    | 2.44                     | 0.81              |
| 2:c:286:THR:OG1   | 2:b:326:LYS:CE   | 2.29                     | 0.81              |
| 2:c:326:LYS:HE2   | 2:d:286:THR:CB   | 2.10                     | 0.81              |
| 1:8:7:DC:C2'      | 2:f:109:ARG:NH1  | 2.43                     | 0.81              |
| 1:8:31:DC:N1      | 2:c:88:ARG:NH1   | 2.28                     | 0.81              |
| 2:e:326:LYS:HE2   | 2:f:286:THR:CB   | 2.09                     | 0.81              |
| 2:c:183:GLY:CA    | 3:c:1000:ADP:H8  | 1.94                     | 0.81              |
| 2:f:183:GLY:CA    | 3:f:1000:ADP:H8  | 1.94                     | 0.80              |
| 1:8:21:DC:H2'     | 2:b:88:ARG:HH11  | 1.46                     | 0.80              |
| 1:8:3:DC:N4       | 2:f:113:LEU:O    | 2.14                     | 0.80              |
| 2:d:183:GLY:CA    | 3:d:1000:ADP:H8  | 1.94                     | 0.80              |
| 2:c:138:PRO:CB    | 2:b:214:GLU:CA   | 2.53                     | 0.80              |
| 2:a:183:GLY:CA    | 3:a:1000:ADP:H8  | 1.93                     | 0.80              |
| 2:b:183:GLY:CA    | 3:b:1000:ADP:H8  | 1.94                     | 0.80              |
| 2:c:184:LYS:CB    | 3:c:1000:ADP:O3B | 2.24                     | 0.80              |
| 1:8:3:DC:O2       | 1:8:3:DC:C3'     | 2.29                     | 0.80              |
| 3:f:1000:ADP:H5'1 | 2:a:366:ARG:NE   | 1.96                     | 0.80              |
| 2:c:218:GLU:CD    | 2:d:140:HIS:HE2  | 1.89                     | 0.80              |
| 2:e:286:THR:HG22  | 2:d:326:LYS:NZ   | 1.89                     | 0.79              |
| 2:f:355:PHE:HE1   | 3:f:1000:ADP:C8  | 2.00                     | 0.79              |
| 2:c:280:ALA:HB2   | 2:d:283:LYS:CD   | 2.13                     | 0.79              |
| 1:8:1:DC:H5'      | 2:f:115:LYS:CD   | 2.12                     | 0.79              |
| 2:e:213:PRO:HB2   | 2:f:138:PRO:CG   | 2.12                     | 0.79              |
| 2:b:355:PHE:HE1   | 3:b:1000:ADP:C8  | 2.01                     | 0.79              |
| 2:d:355:PHE:HE1   | 3:d:1000:ADP:C8  | 2.01                     | 0.79              |
| 2:c:355:PHE:HE1   | 3:c:1000:ADP:C8  | 2.01                     | 0.79              |
| 2:f:347:ARG:NH2   | 2:a:336:LYS:HZ3  | 1.68                     | 0.79              |
| 2:c:286:THR:HG21  | 2:b:326:LYS:NZ   | 1.71                     | 0.79              |
| 1:8:14:DC:H41     | 2:a:102:ARG:NH2  | 1.81                     | 0.78              |
| 2:e:355:PHE:HE1   | 3:e:1000:ADP:C8  | 2.00                     | 0.78              |
| 2:a:355:PHE:HE1   | 3:a:1000:ADP:C8  | 2.01                     | 0.78              |
| 1:8:2:DC:N4       | 2:f:115:LYS:C    | 2.41                     | 0.78              |
| 1:8:23:DC:N4      | 2:b:112:ALA:HB1  | 1.99                     | 0.78              |
| 2:f:184:LYS:CE    | 5:f:1002:BEF:F2  | 2.22                     | 0.78              |
| 2:a:184:LYS:CE    | 5:a:1002:BEF:F2  | 2.22                     | 0.78              |
| 2:d:184:LYS:CE    | 5:d:1002:BEF:F2  | 2.22                     | 0.78              |
| 1:8:21:DC:H1'     | 2:b:88:ARG:CG    | 2.14                     | 0.78              |
| 2:b:138:PRO:CB    | 2:a:214:GLU:HA   | 2.05                     | 0.78              |
| 2:e:347:ARG:NH2   | 2:f:336:LYS:NZ   | 2.31                     | 0.78              |
| 2:e:184:LYS:CE    | 5:e:1002:BEF:F2  | 2.22                     | 0.77              |
| 1:8:3:DC:O2       | 1:8:3:DC:H5''    | 1.84                     | 0.77              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:8:17:DC:C2'     | 2:a:109:ARG:HH12 | 1.97                     | 0.77              |
| 1:8:33:DC:N4      | 2:c:85:GLN:NE2   | 2.23                     | 0.77              |
| 1:8:40:DC:C2      | 2:d:87:ARG:O     | 2.37                     | 0.77              |
| 1:8:53:DC:C5      | 2:e:85:GLN:HG3   | 2.20                     | 0.77              |
| 2:c:184:LYS:CE    | 5:c:1002:BEF:F2  | 2.22                     | 0.77              |
| 1:8:7:DC:H2'      | 2:f:109:ARG:NH1  | 2.00                     | 0.77              |
| 2:e:326:LYS:HE2   | 2:f:286:THR:HG21 | 1.54                     | 0.77              |
| 2:e:286:THR:HB    | 2:d:326:LYS:NZ   | 2.00                     | 0.77              |
| 2:b:184:LYS:CE    | 5:b:1002:BEF:F2  | 2.22                     | 0.77              |
| 2:e:214:GLU:HA    | 2:f:138:PRO:CB   | 2.07                     | 0.77              |
| 2:e:286:THR:HB    | 2:d:326:LYS:HZ1  | 1.50                     | 0.76              |
| 2:d:355:PHE:CE1   | 3:d:1000:ADP:C8  | 2.73                     | 0.76              |
| 2:e:355:PHE:CE1   | 3:e:1000:ADP:C8  | 2.73                     | 0.76              |
| 2:f:355:PHE:CE1   | 3:f:1000:ADP:C8  | 2.73                     | 0.76              |
| 2:e:214:GLU:CB    | 2:f:138:PRO:HB2  | 2.16                     | 0.76              |
| 2:c:280:ALA:HB2   | 2:d:283:LYS:CE   | 2.15                     | 0.76              |
| 2:b:366:ARG:CG    | 3:a:1000:ADP:H4' | 2.16                     | 0.76              |
| 2:b:355:PHE:CE1   | 3:b:1000:ADP:C8  | 2.73                     | 0.75              |
| 2:e:280:ALA:HB2   | 2:f:283:LYS:HD3  | 1.67                     | 0.75              |
| 1:8:4:DC:H6       | 1:8:4:DC:C5'     | 1.98                     | 0.75              |
| 2:c:355:PHE:CE1   | 3:c:1000:ADP:C8  | 2.74                     | 0.75              |
| 1:8:2:DC:H41      | 2:f:115:LYS:C    | 1.95                     | 0.75              |
| 2:e:366:ARG:CG    | 3:d:1000:ADP:H4' | 2.16                     | 0.75              |
| 2:b:332:TYR:CE2   | 2:b:333:GLU:HG3  | 2.22                     | 0.75              |
| 1:8:21:DC:OP1     | 2:b:87:ARG:NH2   | 2.20                     | 0.75              |
| 2:a:355:PHE:CE1   | 3:a:1000:ADP:C8  | 2.74                     | 0.74              |
| 2:d:333:GLU:C     | 2:d:335:PHE:N    | 2.42                     | 0.74              |
| 2:c:181:LYS:HG3   | 2:d:366:ARG:HE   | 1.51                     | 0.74              |
| 2:c:213:PRO:HG2   | 2:d:305:ARG:NH2  | 2.02                     | 0.74              |
| 1:8:54:DC:H6      | 1:8:54:DC:C5'    | 1.99                     | 0.74              |
| 2:f:214:GLU:HA    | 2:a:138:PRO:CB   | 2.08                     | 0.74              |
| 1:8:53:DC:C5      | 2:e:85:GLN:CD    | 2.66                     | 0.74              |
| 2:b:342:GLU:OE1   | 2:a:181:LYS:HD2  | 1.88                     | 0.74              |
| 1:8:57:DC:C3'     | 2:e:109:ARG:NH1  | 2.51                     | 0.74              |
| 2:e:138:PRO:HG3   | 2:d:213:PRO:HB2  | 1.67                     | 0.74              |
| 2:e:232:PHE:CZ    | 2:f:302:GLY:HA3  | 2.22                     | 0.74              |
| 3:f:1000:ADP:H5'1 | 2:a:366:ARG:CZ   | 2.19                     | 0.73              |
| 1:8:1:DC:P        | 2:f:115:LYS:NZ   | 2.61                     | 0.73              |
| 2:e:213:PRO:CB    | 2:f:138:PRO:HG2  | 2.18                     | 0.73              |
| 1:8:44:DC:H6      | 1:8:44:DC:C5'    | 1.98                     | 0.73              |
| 2:e:212:ARG:H     | 2:e:212:ARG:HH11 | 1.35                     | 0.73              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:e:355:PHE:HE1  | 3:e:1000:ADP:N9 | 1.85                     | 0.73              |
| 2:e:181:LYS:HG3  | 2:f:366:ARG:HE  | 1.54                     | 0.73              |
| 3:f:1000:ADP:C4' | 2:a:366:ARG:HD3 | 2.19                     | 0.73              |
| 1:8:21:DC:O2     | 2:b:88:ARG:HG3  | 1.85                     | 0.73              |
| 2:e:342:GLU:OE1  | 2:d:181:LYS:HD2 | 1.88                     | 0.73              |
| 2:c:214:GLU:N    | 2:d:138:PRO:CB  | 2.52                     | 0.73              |
| 2:b:333:GLU:CB   | 2:a:324:GLY:HA3 | 2.18                     | 0.72              |
| 2:f:353:ARG:NH2  | 2:a:364:GLY:HA3 | 2.04                     | 0.72              |
| 2:e:355:PHE:CE1  | 3:e:1000:ADP:C5 | 2.76                     | 0.72              |
| 2:b:333:GLU:HG2  | 2:b:336:LYS:HD2 | 1.69                     | 0.72              |
| 2:b:366:ARG:HE   | 2:a:181:LYS:HG3 | 1.53                     | 0.72              |
| 2:c:342:GLU:OE1  | 2:b:181:LYS:HD2 | 1.88                     | 0.72              |
| 2:d:355:PHE:HE1  | 3:d:1000:ADP:N9 | 1.85                     | 0.72              |
| 3:c:1000:ADP:H4' | 2:d:366:ARG:HG2 | 1.72                     | 0.72              |
| 1:8:1:DC:OP1     | 2:f:115:LYS:CE  | 2.36                     | 0.71              |
| 2:e:286:THR:CB   | 2:d:326:LYS:HE2 | 2.18                     | 0.71              |
| 2:f:213:PRO:CB   | 2:a:138:PRO:HG2 | 2.19                     | 0.71              |
| 2:c:138:PRO:HB2  | 2:b:214:GLU:CB  | 2.19                     | 0.71              |
| 2:c:280:ALA:HB2  | 2:d:283:LYS:HD3 | 1.67                     | 0.71              |
| 2:c:355:PHE:CE1  | 3:c:1000:ADP:C5 | 2.76                     | 0.71              |
| 2:b:355:PHE:HE1  | 3:b:1000:ADP:N9 | 1.85                     | 0.71              |
| 2:c:326:LYS:HZ1  | 2:d:286:THR:CG2 | 1.83                     | 0.71              |
| 2:c:280:ALA:CB   | 2:d:283:LYS:CD  | 2.69                     | 0.71              |
| 1:8:22:DC:H4'    | 1:8:22:DC:OP1   | 1.89                     | 0.71              |
| 2:f:218:GLU:CD   | 2:a:140:HIS:NE2 | 2.46                     | 0.71              |
| 2:f:355:PHE:HE1  | 3:f:1000:ADP:N9 | 1.85                     | 0.71              |
| 2:d:294:LEU:HD13 | 2:d:334:GLU:HG2 | 1.72                     | 0.71              |
| 2:b:138:PRO:CG   | 2:a:213:PRO:C   | 2.62                     | 0.71              |
| 1:8:1:DC:H5      | 2:f:116:VAL:O   | 1.74                     | 0.70              |
| 2:c:214:GLU:CB   | 2:d:138:PRO:HB2 | 2.22                     | 0.70              |
| 1:8:11:DC:H2'    | 2:a:88:ARG:HH11 | 0.54                     | 0.70              |
| 2:f:214:GLU:HB3  | 2:a:138:PRO:CB  | 2.21                     | 0.70              |
| 2:c:138:PRO:HG2  | 2:b:213:PRO:CA  | 2.21                     | 0.70              |
| 1:8:31:DC:C2     | 2:c:88:ARG:NH1  | 2.60                     | 0.70              |
| 2:e:208:LEU:HB3  | 2:e:211:GLU:HG3 | 1.71                     | 0.70              |
| 2:b:333:GLU:HB3  | 2:a:323:THR:O   | 1.92                     | 0.70              |
| 2:c:286:THR:HG22 | 2:b:326:LYS:HZ1 | 1.44                     | 0.70              |
| 2:d:355:PHE:CE1  | 3:d:1000:ADP:C5 | 2.76                     | 0.70              |
| 2:e:212:ARG:HG2  | 2:f:173:ARG:CZ  | 2.21                     | 0.70              |
| 2:b:138:PRO:HG2  | 2:a:213:PRO:CA  | 2.22                     | 0.70              |
| 1:8:41:DC:C1'    | 2:d:88:ARG:NH1  | 2.55                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:f:272:ARG:NH2  | 2:a:334:GLU:OE2  | 2.25                     | 0.69              |
| 2:c:288:GLY:HA3  | 2:d:285:LEU:HG   | 1.73                     | 0.69              |
| 2:b:302:GLY:HA3  | 2:a:232:PHE:CZ   | 2.26                     | 0.69              |
| 2:e:138:PRO:CB   | 2:d:214:GLU:N    | 2.54                     | 0.69              |
| 2:c:276:THR:HG23 | 2:d:292:ASN:OD1  | 1.92                     | 0.69              |
| 3:c:1000:ADP:C5' | 2:d:366:ARG:CD   | 2.70                     | 0.69              |
| 2:c:212:ARG:HG2  | 2:d:173:ARG:NH2  | 2.06                     | 0.69              |
| 2:a:355:PHE:CE1  | 3:a:1000:ADP:C5  | 2.76                     | 0.69              |
| 2:c:333:GLU:CB   | 2:b:324:GLY:HA3  | 2.19                     | 0.69              |
| 2:c:385:LYS:NZ   | 2:b:352:LYS:HG2  | 2.08                     | 0.69              |
| 1:8:40:DC:P      | 2:d:87:ARG:NH1   | 2.66                     | 0.69              |
| 1:8:57:DC:OP2    | 1:8:57:DC:H3'    | 1.92                     | 0.69              |
| 3:e:1000:ADP:H4' | 2:f:366:ARG:CG   | 2.21                     | 0.69              |
| 2:c:138:PRO:O    | 2:b:217:THR:HG21 | 1.92                     | 0.69              |
| 2:c:140:HIS:NE2  | 2:b:218:GLU:CD   | 2.47                     | 0.69              |
| 1:8:40:DC:O2     | 2:d:87:ARG:C     | 2.36                     | 0.69              |
| 2:f:355:PHE:CE1  | 3:f:1000:ADP:C5  | 2.76                     | 0.69              |
| 2:c:347:ARG:HH22 | 2:d:336:LYS:HZ3  | 1.39                     | 0.69              |
| 1:8:23:DC:H41    | 2:b:112:ALA:HB1  | 1.57                     | 0.68              |
| 1:8:41:DC:H1'    | 2:d:88:ARG:HH12  | 1.59                     | 0.68              |
| 2:c:280:ALA:HB2  | 2:d:283:LYS:HE2  | 1.74                     | 0.68              |
| 2:e:213:PRO:HG3  | 2:e:231:THR:HG21 | 1.75                     | 0.68              |
| 2:c:213:PRO:CB   | 2:d:138:PRO:HG2  | 2.23                     | 0.68              |
| 2:e:333:GLU:HB3  | 2:d:323:THR:O    | 1.94                     | 0.68              |
| 1:8:37:DC:OP2    | 1:8:37:DC:H3'    | 1.94                     | 0.68              |
| 2:e:326:LYS:NZ   | 2:f:286:THR:HG21 | 1.85                     | 0.68              |
| 1:8:27:DC:OP2    | 1:8:27:DC:H3'    | 1.94                     | 0.68              |
| 2:f:213:PRO:C    | 2:a:138:PRO:HG2  | 2.18                     | 0.68              |
| 1:8:33:DC:C2     | 2:c:84:SER:OG    | 2.47                     | 0.68              |
| 2:e:305:ARG:CZ   | 2:d:213:PRO:HG2  | 2.22                     | 0.67              |
| 2:c:286:THR:HG21 | 2:b:326:LYS:HE3  | 0.70                     | 0.67              |
| 2:a:355:PHE:HE1  | 3:a:1000:ADP:N9  | 1.85                     | 0.67              |
| 2:e:283:LYS:HD3  | 2:d:280:ALA:CB   | 2.24                     | 0.67              |
| 2:b:355:PHE:CE1  | 3:b:1000:ADP:C5  | 2.76                     | 0.67              |
| 1:8:7:DC:OP2     | 1:8:7:DC:H3'     | 1.94                     | 0.67              |
| 1:8:21:DC:H2'    | 2:b:88:ARG:HD2   | 1.75                     | 0.67              |
| 2:e:138:PRO:HB2  | 2:d:214:GLU:CB   | 2.25                     | 0.67              |
| 2:f:352:LYS:HG2  | 2:a:385:LYS:NZ   | 2.08                     | 0.67              |
| 2:c:218:GLU:OE2  | 2:d:140:HIS:NE2  | 2.22                     | 0.67              |
| 1:8:17:DC:OP2    | 1:8:17:DC:H3'    | 1.94                     | 0.67              |
| 1:8:47:DC:OP2    | 1:8:47:DC:H3'    | 1.94                     | 0.67              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:e:324:GLY:HA3  | 2:f:333:GLU:CG    | 2.24                     | 0.67              |
| 2:c:294:LEU:HD13 | 2:c:334:GLU:HG2   | 1.76                     | 0.67              |
| 2:b:305:ARG:NH2  | 2:a:213:PRO:CG    | 2.50                     | 0.67              |
| 2:f:208:LEU:HB3  | 2:f:211:GLU:HG3   | 1.77                     | 0.67              |
| 2:c:333:GLU:HA   | 2:c:336:LYS:HB2   | 1.75                     | 0.67              |
| 2:c:355:PHE:HE1  | 3:c:1000:ADP:N9   | 1.86                     | 0.66              |
| 2:c:366:ARG:NE   | 3:b:1000:ADP:H5'1 | 2.10                     | 0.66              |
| 2:f:324:GLY:CA   | 2:a:333:GLU:HG3   | 2.25                     | 0.66              |
| 2:e:213:PRO:C    | 2:f:138:PRO:HG2   | 2.21                     | 0.66              |
| 1:8:31:DC:O2     | 2:c:88:ARG:HG3    | 1.96                     | 0.66              |
| 2:e:181:LYS:HD2  | 2:f:342:GLU:OE1   | 1.95                     | 0.66              |
| 3:f:1000:ADP:O1A | 2:a:366:ARG:NH2   | 2.28                     | 0.66              |
| 1:8:1:DC:C6      | 2:f:116:VAL:O     | 2.48                     | 0.66              |
| 2:e:213:PRO:HG2  | 2:f:305:ARG:NH2   | 2.11                     | 0.66              |
| 2:c:333:GLU:HB3  | 2:b:324:GLY:CA    | 2.19                     | 0.66              |
| 1:8:2:DC:C5      | 2:f:115:LYS:CA    | 2.79                     | 0.66              |
| 2:c:173:ARG:HB3  | 2:c:340:ASN:HD21  | 1.59                     | 0.66              |
| 2:e:347:ARG:NH2  | 2:f:336:LYS:HZ1   | 1.93                     | 0.66              |
| 3:f:1000:ADP:C5' | 2:a:366:ARG:NE    | 2.58                     | 0.66              |
| 2:c:213:PRO:HB2  | 2:d:138:PRO:CG    | 2.25                     | 0.66              |
| 2:b:305:ARG:HH22 | 2:a:213:PRO:HG2   | 1.59                     | 0.66              |
| 2:b:185:THR:H    | 3:b:1000:ADP:PA   | 2.19                     | 0.66              |
| 2:d:185:THR:H    | 3:d:1000:ADP:PA   | 2.19                     | 0.66              |
| 2:d:355:PHE:HD1  | 3:d:1000:ADP:C5   | 2.13                     | 0.66              |
| 2:a:184:LYS:H    | 3:a:1000:ADP:PB   | 2.19                     | 0.65              |
| 2:e:347:ARG:HH22 | 2:f:336:LYS:HZ1   | 1.43                     | 0.65              |
| 2:f:355:PHE:HD1  | 3:f:1000:ADP:C5   | 2.14                     | 0.65              |
| 2:e:280:ALA:HB2  | 2:f:283:LYS:CD    | 2.25                     | 0.65              |
| 2:f:185:THR:H    | 3:f:1000:ADP:PA   | 2.19                     | 0.65              |
| 2:c:214:GLU:CA   | 2:d:138:PRO:CB    | 2.59                     | 0.65              |
| 1:8:53:DC:C5     | 2:e:85:GLN:CG     | 2.78                     | 0.65              |
| 2:e:185:THR:H    | 3:e:1000:ADP:PA   | 2.19                     | 0.65              |
| 2:f:184:LYS:H    | 3:f:1000:ADP:PB   | 2.19                     | 0.65              |
| 2:b:333:GLU:HB3  | 2:a:323:THR:C     | 2.22                     | 0.65              |
| 2:a:185:THR:H    | 3:a:1000:ADP:PA   | 2.19                     | 0.65              |
| 2:f:214:GLU:N    | 2:a:138:PRO:HG2   | 2.11                     | 0.65              |
| 2:c:184:LYS:H    | 3:c:1000:ADP:PB   | 2.19                     | 0.65              |
| 2:b:333:GLU:HB2  | 2:a:324:GLY:HA3   | 1.77                     | 0.65              |
| 2:c:185:THR:H    | 3:c:1000:ADP:PA   | 2.19                     | 0.65              |
| 1:8:24:DC:H5''   | 1:8:24:DC:H6      | 1.62                     | 0.65              |
| 2:e:183:GLY:CA   | 3:e:1000:ADP:C8   | 2.80                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:e:184:LYS:H    | 3:e:1000:ADP:PB   | 2.19                     | 0.64              |
| 2:e:288:GLY:HA3  | 2:f:285:LEU:HG    | 1.79                     | 0.64              |
| 2:b:333:GLU:HG2  | 2:b:336:LYS:CD    | 2.27                     | 0.64              |
| 2:d:183:GLY:CA   | 3:d:1000:ADP:C8   | 2.80                     | 0.64              |
| 2:c:347:ARG:NH2  | 2:d:336:LYS:NZ    | 2.45                     | 0.64              |
| 2:e:333:GLU:HB3  | 2:d:324:GLY:CA    | 2.24                     | 0.64              |
| 2:c:355:PHE:CD1  | 3:c:1000:ADP:C6   | 2.85                     | 0.64              |
| 1:8:55:DC:N3     | 2:e:80:TYR:CZ     | 2.66                     | 0.64              |
| 2:e:283:LYS:HD3  | 2:d:280:ALA:HB2   | 1.80                     | 0.64              |
| 2:b:184:LYS:H    | 3:b:1000:ADP:PB   | 2.19                     | 0.64              |
| 2:e:212:ARG:HG2  | 2:f:173:ARG:NH2   | 2.12                     | 0.64              |
| 3:f:1000:ADP:C4' | 2:a:366:ARG:CG    | 2.75                     | 0.64              |
| 2:c:138:PRO:CG   | 2:b:213:PRO:CB    | 2.58                     | 0.64              |
| 2:f:183:GLY:CA   | 3:f:1000:ADP:C8   | 2.80                     | 0.64              |
| 2:b:138:PRO:CB   | 2:a:214:GLU:HB3   | 2.28                     | 0.64              |
| 2:b:355:PHE:CD1  | 3:b:1000:ADP:C6   | 2.86                     | 0.64              |
| 2:c:183:GLY:CA   | 3:c:1000:ADP:C8   | 2.80                     | 0.63              |
| 2:d:184:LYS:H    | 3:d:1000:ADP:PB   | 2.19                     | 0.63              |
| 2:d:355:PHE:CD1  | 3:d:1000:ADP:C6   | 2.85                     | 0.63              |
| 2:e:355:PHE:CD1  | 3:e:1000:ADP:C6   | 2.86                     | 0.63              |
| 2:f:355:PHE:CD1  | 3:f:1000:ADP:C6   | 2.86                     | 0.63              |
| 2:b:183:GLY:CA   | 3:b:1000:ADP:C8   | 2.80                     | 0.63              |
| 2:a:355:PHE:CD1  | 3:a:1000:ADP:C6   | 2.86                     | 0.63              |
| 1:8:2:DC:N4      | 2:f:116:VAL:N     | 2.47                     | 0.63              |
| 1:8:33:DC:O2     | 2:c:82:SER:HB2    | 1.97                     | 0.63              |
| 2:e:140:HIS:NE2  | 2:d:218:GLU:CD    | 2.52                     | 0.63              |
| 2:e:286:THR:HB   | 2:d:326:LYS:CE    | 2.29                     | 0.63              |
| 2:a:183:GLY:CA   | 3:a:1000:ADP:C8   | 2.80                     | 0.63              |
| 2:a:234:GLU:OE2  | 2:a:238:ARG:NH1   | 2.32                     | 0.63              |
| 2:b:292:ASN:OD1  | 2:a:276:THR:HG23  | 1.99                     | 0.63              |
| 1:8:40:DC:O2     | 2:d:87:ARG:CB     | 2.47                     | 0.63              |
| 2:b:333:GLU:HB3  | 2:a:324:GLY:HA3   | 1.79                     | 0.63              |
| 2:b:234:GLU:OE2  | 2:b:238:ARG:NH1   | 2.32                     | 0.63              |
| 2:e:234:GLU:OE2  | 2:e:238:ARG:NH1   | 2.32                     | 0.62              |
| 2:c:280:ALA:CA   | 2:d:283:LYS:HD3   | 2.29                     | 0.62              |
| 2:b:283:LYS:HD3  | 2:a:280:ALA:CB    | 2.29                     | 0.62              |
| 2:b:366:ARG:NE   | 3:a:1000:ADP:H5'1 | 2.14                     | 0.62              |
| 1:8:13:DC:H6     | 1:8:13:DC:H5''    | 1.64                     | 0.62              |
| 1:8:31:DC:C6     | 2:c:88:ARG:NH1    | 2.63                     | 0.62              |
| 2:e:212:ARG:HG3  | 2:e:232:PHE:HE2   | 1.64                     | 0.62              |
| 2:e:294:LEU:HD13 | 2:e:334:GLU:HG2   | 1.80                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:f:214:GLU:CB   | 2:a:138:PRO:CB    | 2.75                     | 0.62              |
| 2:c:336:LYS:HZ3  | 2:b:347:ARG:NH2   | 1.83                     | 0.62              |
| 2:d:333:GLU:O    | 2:d:335:PHE:N     | 2.30                     | 0.62              |
| 2:c:366:ARG:CZ   | 3:b:1000:ADP:H5'1 | 2.30                     | 0.62              |
| 2:a:355:PHE:HD1  | 3:a:1000:ADP:C5   | 2.13                     | 0.62              |
| 2:f:324:GLY:O    | 2:f:326:LYS:N     | 2.33                     | 0.62              |
| 2:d:234:GLU:OE2  | 2:d:238:ARG:NH1   | 2.32                     | 0.62              |
| 1:8:14:DC:N4     | 2:a:102:ARG:NH2   | 2.48                     | 0.62              |
| 1:8:1:DC:N4      | 2:f:116:VAL:CB    | 2.63                     | 0.61              |
| 2:c:138:PRO:CB   | 2:b:214:GLU:HA    | 2.13                     | 0.61              |
| 2:f:181:LYS:HG3  | 2:a:366:ARG:HE    | 1.65                     | 0.61              |
| 2:b:330:VAL:O    | 2:b:334:GLU:HB3   | 1.99                     | 0.61              |
| 2:a:183:GLY:HA2  | 3:a:1000:ADP:PA   | 2.40                     | 0.61              |
| 2:d:321:ILE:HG22 | 2:d:332:TYR:CD2   | 2.34                     | 0.61              |
| 2:f:272:ARG:HH22 | 2:a:334:GLU:CD    | 2.08                     | 0.61              |
| 2:e:138:PRO:O    | 2:d:217:THR:HG21  | 2.00                     | 0.61              |
| 2:e:217:THR:HG21 | 2:f:138:PRO:O     | 2.01                     | 0.61              |
| 2:c:366:ARG:HE   | 2:b:181:LYS:HG3   | 1.64                     | 0.61              |
| 2:e:280:ALA:HB2  | 2:f:283:LYS:CE    | 2.29                     | 0.61              |
| 2:f:332:TYR:CE2  | 2:f:333:GLU:HG2   | 2.35                     | 0.61              |
| 2:c:234:GLU:OE2  | 2:c:238:ARG:NH1   | 2.32                     | 0.61              |
| 2:b:138:PRO:HG2  | 2:a:214:GLU:N     | 2.14                     | 0.61              |
| 1:8:55:DC:C2     | 2:e:80:TYR:CZ     | 2.89                     | 0.61              |
| 1:8:2:DC:N4      | 2:f:115:LYS:N     | 2.37                     | 0.61              |
| 2:e:212:ARG:HG3  | 2:e:232:PHE:CE2   | 2.36                     | 0.61              |
| 2:e:366:ARG:CB   | 3:d:1000:ADP:HO3' | 1.93                     | 0.61              |
| 2:f:183:GLY:HA2  | 3:f:1000:ADP:PA   | 2.41                     | 0.61              |
| 2:c:183:GLY:CA   | 3:c:1000:ADP:PA   | 2.89                     | 0.61              |
| 2:c:232:PHE:CE1  | 2:d:302:GLY:HA3   | 2.34                     | 0.61              |
| 2:c:366:ARG:NH2  | 3:b:1000:ADP:O2A  | 2.34                     | 0.61              |
| 2:b:183:GLY:CA   | 3:b:1000:ADP:PA   | 2.89                     | 0.61              |
| 2:a:183:GLY:CA   | 3:a:1000:ADP:PA   | 2.89                     | 0.61              |
| 1:8:2:DC:H41     | 2:f:114:LEU:C     | 2.08                     | 0.61              |
| 2:e:366:ARG:HE   | 2:d:181:LYS:HG3   | 1.66                     | 0.61              |
| 2:f:181:LYS:CD   | 2:a:342:GLU:OE1   | 2.46                     | 0.61              |
| 2:f:272:ARG:NH1  | 2:a:334:GLU:CD    | 2.34                     | 0.61              |
| 3:f:1000:ADP:C4' | 2:a:366:ARG:CD    | 2.77                     | 0.61              |
| 2:c:355:PHE:HD1  | 3:c:1000:ADP:C5   | 2.13                     | 0.60              |
| 2:b:355:PHE:CZ   | 3:b:1000:ADP:H1'  | 2.36                     | 0.60              |
| 1:8:31:DC:H2'    | 2:c:88:ARG:NH1    | 2.16                     | 0.60              |
| 2:c:355:PHE:CZ   | 3:c:1000:ADP:H1'  | 2.36                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:8:21:DC:O2     | 2:b:88:ARG:HG2    | 2.01                     | 0.60              |
| 2:f:234:GLU:OE2  | 2:f:238:ARG:NH1   | 2.32                     | 0.60              |
| 2:b:183:GLY:HA2  | 3:b:1000:ADP:PA   | 2.41                     | 0.60              |
| 1:8:3:DC:O2      | 1:8:3:DC:C4'      | 2.50                     | 0.60              |
| 2:e:183:GLY:CA   | 3:e:1000:ADP:PA   | 2.89                     | 0.60              |
| 2:f:183:GLY:CA   | 3:f:1000:ADP:PA   | 2.89                     | 0.60              |
| 2:c:347:ARG:HH22 | 2:d:336:LYS:HZ1   | 1.50                     | 0.60              |
| 2:d:183:GLY:HA2  | 3:d:1000:ADP:PA   | 2.41                     | 0.60              |
| 1:8:38:DC:O2     | 1:8:38:DC:C2'     | 2.50                     | 0.60              |
| 2:c:183:GLY:HA2  | 3:c:1000:ADP:PA   | 2.41                     | 0.60              |
| 2:b:355:PHE:HD1  | 3:b:1000:ADP:C5   | 2.13                     | 0.60              |
| 2:a:183:GLY:HA3  | 3:a:1000:ADP:C8   | 2.37                     | 0.60              |
| 2:f:355:PHE:CZ   | 3:f:1000:ADP:H1'  | 2.36                     | 0.60              |
| 2:d:183:GLY:CA   | 3:d:1000:ADP:PA   | 2.89                     | 0.60              |
| 1:8:3:DC:O2      | 1:8:3:DC:C5'      | 2.50                     | 0.60              |
| 2:e:355:PHE:CZ   | 3:e:1000:ADP:H1'  | 2.36                     | 0.60              |
| 2:c:138:PRO:CG   | 2:b:213:PRO:C     | 2.69                     | 0.60              |
| 2:b:333:GLU:C    | 2:b:336:LYS:H     | 2.09                     | 0.60              |
| 2:b:336:LYS:HZ1  | 2:a:347:ARG:HH22  | 1.18                     | 0.60              |
| 1:8:31:DC:H2'    | 2:c:88:ARG:HH11   | 1.67                     | 0.59              |
| 2:e:326:LYS:HZ1  | 2:f:286:THR:CB    | 2.14                     | 0.59              |
| 2:f:329:GLU:O    | 2:f:333:GLU:HB2   | 2.02                     | 0.59              |
| 2:e:184:LYS:HE3  | 5:e:1002:BEF:F2   | 1.92                     | 0.59              |
| 2:a:355:PHE:CZ   | 3:a:1000:ADP:H1'  | 2.37                     | 0.59              |
| 2:c:213:PRO:HG3  | 2:c:231:THR:HG21  | 1.84                     | 0.59              |
| 2:c:286:THR:CG2  | 2:b:326:LYS:HZ2   | 2.08                     | 0.59              |
| 2:b:184:LYS:HE3  | 5:b:1002:BEF:F2   | 1.92                     | 0.59              |
| 2:d:183:GLY:HA3  | 3:d:1000:ADP:C8   | 2.37                     | 0.59              |
| 1:8:2:DC:N4      | 2:f:114:LEU:C     | 2.59                     | 0.59              |
| 1:8:21:DC:N1     | 2:b:88:ARG:NH1    | 2.49                     | 0.59              |
| 2:e:138:PRO:HG2  | 2:d:213:PRO:CA    | 2.32                     | 0.59              |
| 2:e:272:ARG:HH22 | 2:f:334:GLU:CD    | 2.10                     | 0.59              |
| 2:f:214:GLU:N    | 2:a:138:PRO:CG    | 2.66                     | 0.59              |
| 2:b:183:GLY:HA3  | 3:b:1000:ADP:C8   | 2.37                     | 0.59              |
| 2:e:366:ARG:NE   | 3:d:1000:ADP:H5'1 | 2.17                     | 0.59              |
| 2:f:184:LYS:HE3  | 5:f:1002:BEF:F2   | 1.92                     | 0.59              |
| 2:e:183:GLY:HA2  | 3:e:1000:ADP:PA   | 2.41                     | 0.59              |
| 1:8:3:DC:N4      | 2:f:114:LEU:HD13  | 2.17                     | 0.59              |
| 2:e:218:GLU:CD   | 2:f:140:HIS:NE2   | 2.55                     | 0.59              |
| 2:d:355:PHE:CZ   | 3:d:1000:ADP:H1'  | 2.37                     | 0.59              |
| 2:e:183:GLY:HA3  | 3:e:1000:ADP:C8   | 2.38                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:f:183:GLY:HA3  | 3:f:1000:ADP:C8   | 2.37                     | 0.59              |
| 2:f:217:THR:HG21 | 2:a:138:PRO:O     | 2.03                     | 0.59              |
| 2:b:333:GLU:O    | 2:b:336:LYS:N     | 2.35                     | 0.59              |
| 1:8:33:DC:H5''   | 1:8:33:DC:H6      | 1.67                     | 0.58              |
| 2:e:214:GLU:HB3  | 2:f:138:PRO:CB    | 2.32                     | 0.58              |
| 2:f:325:SER:O    | 2:f:327:MET:N     | 2.36                     | 0.58              |
| 1:8:53:DC:C5     | 2:e:82:SER:OG     | 2.54                     | 0.58              |
| 2:a:16:THR:O     | 2:a:20:ASN:ND2    | 2.33                     | 0.58              |
| 2:f:184:LYS:N    | 3:f:1000:ADP:PA   | 2.76                     | 0.58              |
| 2:c:212:ARG:CZ   | 2:d:173:ARG:HH21  | 2.16                     | 0.58              |
| 2:a:184:LYS:HE3  | 5:a:1002:BEF:F2   | 1.92                     | 0.58              |
| 2:d:184:LYS:HE3  | 5:d:1002:BEF:F2   | 1.92                     | 0.58              |
| 1:8:58:DC:P      | 2:e:109:ARG:HH12  | 2.27                     | 0.58              |
| 2:b:184:LYS:HB2  | 3:b:1000:ADP:PB   | 2.43                     | 0.58              |
| 2:e:366:ARG:HH11 | 2:d:181:LYS:HA    | 0.82                     | 0.58              |
| 2:c:184:LYS:N    | 3:c:1000:ADP:PA   | 2.76                     | 0.58              |
| 2:c:280:ALA:HA   | 2:d:283:LYS:HD3   | 1.84                     | 0.58              |
| 2:c:366:ARG:HD3  | 3:b:1000:ADP:C4'  | 2.33                     | 0.58              |
| 2:c:184:LYS:HE3  | 5:c:1002:BEF:F2   | 1.93                     | 0.58              |
| 2:c:183:GLY:HA3  | 3:c:1000:ADP:C8   | 2.38                     | 0.58              |
| 2:c:324:GLY:HA3  | 2:d:333:GLU:CG    | 2.34                     | 0.58              |
| 2:c:347:ARG:NH2  | 2:d:336:LYS:HZ1   | 2.02                     | 0.58              |
| 1:8:11:DC:C3'    | 2:a:88:ARG:NH1    | 2.64                     | 0.58              |
| 2:f:288:GLY:HA3  | 2:a:285:LEU:HG    | 1.86                     | 0.58              |
| 2:c:232:PHE:CZ   | 2:d:302:GLY:CA    | 2.87                     | 0.58              |
| 1:8:7:DC:O2      | 2:f:109:ARG:NH2   | 2.36                     | 0.57              |
| 2:e:181:LYS:CB   | 2:f:366:ARG:NH1   | 2.61                     | 0.57              |
| 2:b:366:ARG:CZ   | 3:a:1000:ADP:H5'1 | 2.34                     | 0.57              |
| 2:d:184:LYS:N    | 3:d:1000:ADP:PA   | 2.76                     | 0.57              |
| 2:b:302:GLY:O    | 2:a:232:PHE:HZ    | 1.87                     | 0.57              |
| 2:a:184:LYS:N    | 3:a:1000:ADP:PA   | 2.76                     | 0.57              |
| 1:8:24:DC:N4     | 2:b:108:GLU:OE2   | 2.37                     | 0.57              |
| 2:e:184:LYS:N    | 3:e:1000:ADP:PA   | 2.76                     | 0.57              |
| 2:e:326:LYS:NZ   | 2:f:286:THR:CB    | 2.64                     | 0.57              |
| 2:c:212:ARG:NH2  | 2:c:215:GLU:OE2   | 2.37                     | 0.57              |
| 2:b:138:PRO:O    | 2:a:217:THR:HG21  | 2.04                     | 0.57              |
| 2:a:184:LYS:HB2  | 3:a:1000:ADP:PB   | 2.44                     | 0.57              |
| 1:8:2:DC:O2      | 2:f:89:PHE:CE2    | 2.41                     | 0.57              |
| 2:e:355:PHE:HD1  | 3:e:1000:ADP:C5   | 2.13                     | 0.57              |
| 2:b:366:ARG:HD3  | 3:a:1000:ADP:C4'  | 2.33                     | 0.57              |
| 2:d:16:THR:O     | 2:d:20:ASN:ND2    | 2.33                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:8:1:DC:H2'     | 1:8:1:DC:O2      | 2.04                     | 0.57              |
| 2:b:184:LYS:N    | 3:b:1000:ADP:PA  | 2.76                     | 0.57              |
| 1:8:21:DC:C2'    | 2:b:88:ARG:HH11  | 2.17                     | 0.57              |
| 2:e:366:ARG:NH2  | 3:d:1000:ADP:O1A | 2.38                     | 0.57              |
| 2:c:366:ARG:NH1  | 2:b:181:LYS:CB   | 2.60                     | 0.57              |
| 2:b:138:PRO:CG   | 2:a:214:GLU:N    | 2.66                     | 0.57              |
| 1:8:53:DC:H5     | 2:e:85:GLN:CD    | 2.11                     | 0.57              |
| 1:8:57:DC:H2'    | 2:e:109:ARG:NH1  | 2.11                     | 0.56              |
| 2:b:333:GLU:HA   | 2:b:336:LYS:CB   | 2.33                     | 0.56              |
| 1:8:14:DC:H5''   | 1:8:14:DC:H6     | 1.69                     | 0.56              |
| 1:8:40:DC:O2     | 2:d:87:ARG:HB3   | 2.04                     | 0.56              |
| 3:e:1000:ADP:O1B | 2:f:366:ARG:NH2  | 2.32                     | 0.56              |
| 2:b:138:PRO:CB   | 2:a:214:GLU:CB   | 2.79                     | 0.56              |
| 2:b:366:ARG:NH2  | 3:a:1000:ADP:O2A | 2.38                     | 0.56              |
| 2:b:294:LEU:HD13 | 2:b:334:GLU:HG2  | 1.86                     | 0.56              |
| 1:8:53:DC:H6     | 2:e:84:SER:OG    | 1.88                     | 0.56              |
| 2:d:266:SER:HB2  | 2:d:269:ARG:HB2  | 1.88                     | 0.56              |
| 1:8:34:DC:N3     | 2:c:80:TYR:CZ    | 2.73                     | 0.56              |
| 2:e:214:GLU:N    | 2:f:138:PRO:HG2  | 2.20                     | 0.56              |
| 2:c:16:THR:O     | 2:c:20:ASN:ND2   | 2.32                     | 0.56              |
| 2:c:287:GLY:HA2  | 2:d:286:THR:OG1  | 2.06                     | 0.56              |
| 2:b:333:GLU:C    | 2:a:323:THR:O    | 2.49                     | 0.56              |
| 1:8:21:DC:H1'    | 2:b:88:ARG:CB    | 2.36                     | 0.56              |
| 2:e:355:PHE:CZ   | 3:e:1000:ADP:C4  | 2.92                     | 0.56              |
| 2:f:266:SER:HB2  | 2:f:269:ARG:HB2  | 1.88                     | 0.56              |
| 2:e:212:ARG:HA   | 2:e:232:PHE:HE2  | 1.71                     | 0.56              |
| 2:b:283:LYS:CE   | 2:a:280:ALA:HB2  | 2.36                     | 0.56              |
| 2:c:213:PRO:C    | 2:d:138:PRO:HG2  | 2.31                     | 0.56              |
| 1:8:40:DC:O2     | 2:d:87:ARG:HG2   | 2.05                     | 0.55              |
| 2:c:232:PHE:HZ   | 2:d:302:GLY:O    | 1.88                     | 0.55              |
| 2:b:140:HIS:NE2  | 2:a:218:GLU:CD   | 2.58                     | 0.55              |
| 1:8:1:DC:C6      | 2:f:116:VAL:HG13 | 2.13                     | 0.55              |
| 1:8:58:DC:H5''   | 2:e:109:ARG:CZ   | 2.36                     | 0.55              |
| 2:e:347:ARG:NH2  | 2:f:336:LYS:HZ3  | 1.96                     | 0.55              |
| 2:f:16:THR:O     | 2:f:20:ASN:ND2   | 2.33                     | 0.55              |
| 2:f:213:PRO:HG3  | 2:f:231:THR:HG21 | 1.88                     | 0.55              |
| 2:a:266:SER:HB2  | 2:a:269:ARG:HB2  | 1.88                     | 0.55              |
| 2:d:329:GLU:O    | 2:d:333:GLU:HB2  | 2.07                     | 0.55              |
| 1:8:21:DC:C2     | 2:b:88:ARG:HG2   | 2.40                     | 0.55              |
| 1:8:30:DC:H4'    | 2:c:87:ARG:NH2   | 2.21                     | 0.55              |
| 2:c:355:PHE:CZ   | 3:c:1000:ADP:C4  | 2.92                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:b:266:SER:HB2   | 2:b:269:ARG:HB2  | 1.88                     | 0.55              |
| 2:e:138:PRO:CB    | 2:d:214:GLU:CA   | 2.65                     | 0.55              |
| 2:c:266:SER:HB2   | 2:c:269:ARG:HB2  | 1.88                     | 0.55              |
| 1:8:1:DC:H5       | 2:f:116:VAL:C    | 2.14                     | 0.55              |
| 2:c:184:LYS:HB2   | 3:c:1000:ADP:PB  | 2.44                     | 0.55              |
| 1:8:55:DC:N3      | 2:e:80:TYR:CE1   | 2.75                     | 0.55              |
| 2:e:184:LYS:HB2   | 3:e:1000:ADP:PB  | 2.43                     | 0.55              |
| 3:e:1000:ADP:H5'1 | 2:f:366:ARG:NE   | 2.21                     | 0.55              |
| 2:c:138:PRO:CB    | 2:b:214:GLU:HB3  | 2.36                     | 0.55              |
| 2:c:366:ARG:NE    | 3:b:1000:ADP:C5' | 2.68                     | 0.55              |
| 2:b:16:THR:O      | 2:b:20:ASN:ND2   | 2.33                     | 0.55              |
| 2:c:212:ARG:HD3   | 2:c:215:GLU:OE2  | 2.06                     | 0.55              |
| 2:e:266:SER:HB2   | 2:e:269:ARG:HB2  | 1.88                     | 0.54              |
| 2:b:355:PHE:CZ    | 3:b:1000:ADP:C4  | 2.92                     | 0.54              |
| 1:8:11:DC:H2'     | 2:a:88:ARG:CZ    | 2.20                     | 0.54              |
| 2:d:355:PHE:CZ    | 3:d:1000:ADP:C4  | 2.92                     | 0.54              |
| 1:8:2:DC:H3'      | 1:8:2:DC:H6      | 1.73                     | 0.54              |
| 2:e:16:THR:O      | 2:e:20:ASN:ND2   | 2.33                     | 0.54              |
| 2:f:212:ARG:HA    | 2:f:232:PHE:HE2  | 1.72                     | 0.54              |
| 2:f:333:GLU:O     | 2:f:334:GLU:C    | 2.49                     | 0.54              |
| 2:c:214:GLU:HB3   | 2:d:138:PRO:CB   | 2.38                     | 0.54              |
| 2:c:364:GLY:HA3   | 2:b:353:ARG:NH2  | 2.22                     | 0.54              |
| 2:b:286:THR:OG1   | 2:a:287:GLY:HA2  | 2.07                     | 0.54              |
| 1:8:1:DC:OP1      | 2:f:115:LYS:NZ   | 2.41                     | 0.54              |
| 1:8:53:DC:H5      | 2:e:85:GLN:HG3   | 1.73                     | 0.54              |
| 2:f:213:PRO:HG2   | 2:a:305:ARG:NH2  | 2.23                     | 0.54              |
| 2:e:366:ARG:NH2   | 3:d:1000:ADP:O2B | 2.34                     | 0.53              |
| 1:8:31:DC:C1'     | 2:c:88:ARG:HH11  | 2.22                     | 0.53              |
| 1:8:44:DC:O2      | 2:d:80:TYR:OH    | 2.20                     | 0.53              |
| 1:8:55:DC:O2      | 2:e:80:TYR:CE1   | 2.61                     | 0.53              |
| 2:e:214:GLU:CB    | 2:f:138:PRO:CB   | 2.84                     | 0.53              |
| 2:f:184:LYS:HB2   | 3:f:1000:ADP:PB  | 2.43                     | 0.53              |
| 2:c:217:THR:HG21  | 2:d:138:PRO:O    | 2.08                     | 0.53              |
| 2:c:302:GLY:HA3   | 2:b:232:PHE:CZ   | 2.44                     | 0.53              |
| 2:e:286:THR:HG21  | 2:d:326:LYS:HE3  | 0.54                     | 0.53              |
| 2:b:283:LYS:HE2   | 2:a:280:ALA:HB2  | 1.90                     | 0.53              |
| 2:e:232:PHE:HZ    | 2:f:302:GLY:O    | 1.92                     | 0.53              |
| 2:e:333:GLU:HA    | 2:e:336:LYS:HB3  | 1.91                     | 0.53              |
| 1:8:31:DC:C2'     | 2:c:88:ARG:HH11  | 2.22                     | 0.53              |
| 2:e:302:GLY:HA3   | 2:d:232:PHE:CZ   | 2.43                     | 0.53              |
| 1:8:57:DC:H2''    | 2:e:109:ARG:NH2  | 2.24                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:f:319:ALA:HB1  | 2:f:332:TYR:HB2  | 1.90                     | 0.53              |
| 3:f:1000:ADP:H4' | 2:a:366:ARG:CD   | 2.36                     | 0.53              |
| 2:c:212:ARG:HD3  | 2:c:215:GLU:CD   | 2.34                     | 0.53              |
| 3:e:1000:ADP:O1A | 2:f:366:ARG:NH2  | 2.42                     | 0.53              |
| 3:f:1000:ADP:C5' | 2:a:366:ARG:CZ   | 2.87                     | 0.53              |
| 2:c:333:GLU:C    | 2:c:336:LYS:H    | 2.16                     | 0.53              |
| 2:e:333:GLU:C    | 2:e:336:LYS:H    | 2.17                     | 0.52              |
| 2:a:379:LYS:HD3  | 2:a:413:PHE:HB3  | 1.91                     | 0.52              |
| 1:8:11:DC:H6     | 1:8:11:DC:H3'    | 1.75                     | 0.52              |
| 2:e:379:LYS:HD3  | 2:e:413:PHE:HB3  | 1.92                     | 0.52              |
| 2:f:214:GLU:HB3  | 2:a:138:PRO:HB2  | 1.82                     | 0.52              |
| 2:f:333:GLU:O    | 2:f:336:LYS:N    | 2.28                     | 0.52              |
| 2:b:379:LYS:HD3  | 2:b:413:PHE:HB3  | 1.91                     | 0.52              |
| 2:d:184:LYS:HB2  | 3:d:1000:ADP:PB  | 2.43                     | 0.52              |
| 1:8:21:DC:O2     | 2:b:88:ARG:HA    | 2.09                     | 0.52              |
| 2:e:280:ALA:HB1  | 2:f:283:LYS:HD3  | 1.90                     | 0.52              |
| 2:f:324:GLY:H    | 2:a:333:GLU:CG   | 2.21                     | 0.52              |
| 2:d:379:LYS:HD3  | 2:d:413:PHE:HB3  | 1.91                     | 0.52              |
| 1:8:1:DC:H41     | 2:f:116:VAL:CB   | 2.14                     | 0.52              |
| 2:d:184:LYS:N    | 3:d:1000:ADP:O3A | 2.43                     | 0.52              |
| 2:f:325:SER:C    | 2:f:327:MET:N    | 2.66                     | 0.52              |
| 2:c:138:PRO:O    | 2:b:217:THR:CG2  | 2.57                     | 0.52              |
| 1:8:2:DC:C3'     | 1:8:2:DC:C6      | 2.93                     | 0.52              |
| 2:c:285:LEU:HG   | 2:b:288:GLY:HA3  | 1.91                     | 0.52              |
| 2:d:332:TYR:O    | 2:d:335:PHE:HB2  | 2.10                     | 0.52              |
| 2:e:290:ASP:HB3  | 2:e:293:ALA:HB2  | 1.93                     | 0.51              |
| 2:c:379:LYS:HD3  | 2:c:413:PHE:HB3  | 1.92                     | 0.51              |
| 2:e:138:PRO:CB   | 2:d:214:GLU:HB3  | 2.40                     | 0.51              |
| 2:b:290:ASP:HB3  | 2:b:293:ALA:HB2  | 1.93                     | 0.51              |
| 2:a:184:LYS:N    | 3:a:1000:ADP:O3A | 2.42                     | 0.51              |
| 2:e:213:PRO:HG3  | 2:e:231:THR:CG2  | 2.40                     | 0.51              |
| 2:e:326:LYS:CE   | 2:f:286:THR:HB   | 2.35                     | 0.51              |
| 2:f:290:ASP:HB3  | 2:f:293:ALA:HB2  | 1.93                     | 0.51              |
| 2:f:379:LYS:HD3  | 2:f:413:PHE:HB3  | 1.92                     | 0.51              |
| 2:c:338:THR:O    | 2:c:339:GLY:C    | 2.53                     | 0.51              |
| 3:c:1000:ADP:H4' | 2:d:366:ARG:CG   | 2.39                     | 0.51              |
| 2:c:138:PRO:CG   | 2:b:214:GLU:N    | 2.74                     | 0.51              |
| 1:8:40:DC:O2     | 2:d:87:ARG:CG    | 2.59                     | 0.51              |
| 2:e:214:GLU:N    | 2:f:138:PRO:CG   | 2.72                     | 0.51              |
| 2:f:323:THR:C    | 2:f:325:SER:N    | 2.68                     | 0.51              |
| 2:e:326:LYS:NZ   | 2:f:286:THR:HB   | 2.26                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:c:290:ASP:HB3  | 2:c:293:ALA:HB2  | 1.93                     | 0.51              |
| 2:c:336:LYS:C    | 2:c:338:THR:H    | 2.18                     | 0.51              |
| 1:8:14:DC:H41    | 2:a:102:ARG:HH22 | 1.57                     | 0.50              |
| 1:8:58:DC:P      | 2:e:109:ARG:NH1  | 2.85                     | 0.50              |
| 2:b:138:PRO:CG   | 2:a:213:PRO:CB   | 2.64                     | 0.50              |
| 2:c:352:LYS:CG   | 2:d:385:LYS:NZ   | 2.57                     | 0.50              |
| 1:8:1:DC:C5      | 2:f:116:VAL:CB   | 2.90                     | 0.50              |
| 2:c:138:PRO:HG2  | 2:b:214:GLU:N    | 2.23                     | 0.50              |
| 2:b:289:VAL:HG22 | 2:b:327:MET:HG3  | 1.94                     | 0.50              |
| 2:a:355:PHE:CZ   | 3:a:1000:ADP:C4  | 2.93                     | 0.50              |
| 2:d:289:VAL:HG22 | 2:d:327:MET:HG3  | 1.93                     | 0.50              |
| 1:8:17:DC:C2'    | 2:a:109:ARG:NH1  | 2.71                     | 0.50              |
| 2:e:286:THR:OG1  | 2:d:326:LYS:HE2  | 2.11                     | 0.50              |
| 2:c:289:VAL:HG22 | 2:c:327:MET:HG3  | 1.94                     | 0.50              |
| 1:8:11:DC:C5     | 2:a:88:ARG:NH2   | 2.80                     | 0.50              |
| 1:8:21:DC:H1'    | 2:b:88:ARG:HB2   | 1.93                     | 0.50              |
| 2:f:289:VAL:HG22 | 2:f:327:MET:HG3  | 1.93                     | 0.50              |
| 2:f:355:PHE:CZ   | 3:f:1000:ADP:C4  | 2.93                     | 0.50              |
| 1:8:33:DC:H5''   | 1:8:33:DC:C6     | 2.46                     | 0.50              |
| 2:e:232:PHE:CE1  | 2:f:302:GLY:HA3  | 2.46                     | 0.50              |
| 2:e:289:VAL:HG22 | 2:e:327:MET:HG3  | 1.94                     | 0.50              |
| 2:e:364:GLY:HA3  | 2:d:353:ARG:NH2  | 2.27                     | 0.50              |
| 2:f:184:LYS:N    | 3:f:1000:ADP:O3A | 2.43                     | 0.49              |
| 2:c:333:GLU:HA   | 2:c:336:LYS:CB   | 2.42                     | 0.49              |
| 2:c:183:GLY:CA   | 3:c:1000:ADP:O5' | 2.56                     | 0.49              |
| 2:c:212:ARG:HH12 | 2:d:340:ASN:HB3  | 1.77                     | 0.49              |
| 2:a:289:VAL:HG22 | 2:a:327:MET:HG3  | 1.93                     | 0.49              |
| 2:a:290:ASP:HB3  | 2:a:293:ALA:HB2  | 1.93                     | 0.49              |
| 1:8:17:DC:H2'    | 2:a:109:ARG:NH1  | 2.26                     | 0.49              |
| 1:8:31:DC:H3'    | 1:8:31:DC:H6     | 1.76                     | 0.49              |
| 2:e:183:GLY:N    | 3:e:1000:ADP:O3A | 2.41                     | 0.49              |
| 2:c:181:LYS:HD2  | 2:d:342:GLU:OE1  | 2.12                     | 0.49              |
| 2:c:184:LYS:HG3  | 3:c:1000:ADP:PB  | 2.48                     | 0.49              |
| 2:d:290:ASP:HB3  | 2:d:293:ALA:HB2  | 1.93                     | 0.49              |
| 2:c:333:GLU:C    | 2:b:323:THR:O    | 2.55                     | 0.49              |
| 1:8:33:DC:C4     | 2:c:85:GLN:HG3   | 2.48                     | 0.49              |
| 2:e:326:LYS:HE2  | 2:f:286:THR:HB   | 1.91                     | 0.49              |
| 2:c:214:GLU:HB3  | 2:d:138:PRO:HB2  | 1.94                     | 0.49              |
| 1:8:14:DC:H41    | 2:a:102:ARG:HH21 | 1.58                     | 0.49              |
| 1:8:33:DC:H6     | 1:8:33:DC:C5'    | 2.26                     | 0.49              |
| 2:f:183:GLY:N    | 3:f:1000:ADP:O3A | 2.41                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:f:181:LYS:CE    | 2:a:342:GLU:OE1  | 2.60                     | 0.49              |
| 2:f:353:ARG:HH22  | 2:a:364:GLY:HA3  | 1.78                     | 0.49              |
| 2:d:328:ASP:O     | 2:d:332:TYR:HB3  | 2.13                     | 0.49              |
| 3:e:1000:ADP:H5'1 | 2:f:366:ARG:CD   | 2.42                     | 0.49              |
| 2:c:366:ARG:CD    | 3:b:1000:ADP:C4' | 2.91                     | 0.49              |
| 2:a:183:GLY:N     | 3:a:1000:ADP:O3A | 2.41                     | 0.49              |
| 2:c:333:GLU:O     | 2:c:336:LYS:N    | 2.41                     | 0.49              |
| 2:c:333:GLU:HG3   | 2:c:336:LYS:CD   | 2.43                     | 0.49              |
| 1:8:52:DC:C5      | 2:e:88:ARG:NH2   | 2.81                     | 0.48              |
| 2:c:286:THR:OG1   | 2:b:326:LYS:HE3  | 2.03                     | 0.48              |
| 1:8:2:DC:H3'      | 1:8:2:DC:C6      | 2.47                     | 0.48              |
| 1:8:3:DC:C5       | 2:f:85:GLN:NE2   | 2.81                     | 0.48              |
| 2:f:324:GLY:C     | 2:f:326:LYS:N    | 2.71                     | 0.48              |
| 2:f:333:GLU:C     | 2:f:335:PHE:N    | 2.69                     | 0.48              |
| 2:c:184:LYS:N     | 3:c:1000:ADP:O3A | 2.43                     | 0.48              |
| 2:c:214:GLU:N     | 2:d:138:PRO:HG2  | 2.28                     | 0.48              |
| 3:c:1000:ADP:H5'2 | 2:d:366:ARG:CD   | 2.17                     | 0.48              |
| 2:b:366:ARG:NH2   | 3:a:1000:ADP:O2B | 2.38                     | 0.48              |
| 2:e:184:LYS:HG3   | 3:e:1000:ADP:PB  | 2.49                     | 0.48              |
| 2:e:336:LYS:HD3   | 2:d:180:PRO:CG   | 2.43                     | 0.48              |
| 2:c:333:GLU:HG3   | 2:c:336:LYS:HD2  | 1.95                     | 0.48              |
| 2:e:272:ARG:NH2   | 2:f:334:GLU:CD   | 2.61                     | 0.48              |
| 2:a:183:GLY:HA2   | 3:a:1000:ADP:C8  | 2.35                     | 0.48              |
| 1:8:1:DC:OP1      | 1:8:1:DC:H4'     | 2.14                     | 0.48              |
| 2:e:138:PRO:HB2   | 2:d:214:GLU:HB3  | 1.96                     | 0.48              |
| 2:f:184:LYS:HG3   | 3:f:1000:ADP:PB  | 2.49                     | 0.48              |
| 1:8:23:DC:H5''    | 1:8:23:DC:O2     | 2.13                     | 0.48              |
| 1:8:53:DC:H5      | 2:e:85:GLN:CG    | 2.27                     | 0.48              |
| 2:f:324:GLY:H     | 2:a:333:GLU:CD   | 2.22                     | 0.48              |
| 2:e:232:PHE:CZ    | 2:f:302:GLY:CA   | 2.96                     | 0.47              |
| 2:b:184:LYS:N     | 3:b:1000:ADP:O3A | 2.43                     | 0.47              |
| 2:e:333:GLU:HB3   | 2:d:323:THR:C    | 2.38                     | 0.47              |
| 2:e:366:ARG:NE    | 3:d:1000:ADP:C5' | 2.76                     | 0.47              |
| 2:f:183:GLY:C     | 3:f:1000:ADP:PA  | 2.97                     | 0.47              |
| 2:c:67:SER:OG     | 2:c:69:ASP:OD1   | 2.32                     | 0.47              |
| 2:c:138:PRO:CB    | 2:b:214:GLU:CB   | 2.88                     | 0.47              |
| 2:b:183:GLY:N     | 3:b:1000:ADP:O3A | 2.41                     | 0.47              |
| 1:8:21:DC:C1'     | 2:b:88:ARG:CG    | 2.70                     | 0.47              |
| 2:e:339:GLY:H     | 2:d:212:ARG:NH2  | 2.12                     | 0.47              |
| 2:e:217:THR:CG2   | 2:f:138:PRO:O    | 2.63                     | 0.47              |
| 2:f:212:ARG:HH12  | 2:a:338:THR:HG22 | 1.79                     | 0.47              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:b:355:PHE:CE1 | 3:b:1000:ADP:C1' | 2.98                     | 0.47              |
| 2:d:183:GLY:CA  | 3:d:1000:ADP:O5' | 2.56                     | 0.47              |
| 1:8:1:DC:C5'    | 2:f:115:LYS:CD   | 2.80                     | 0.47              |
| 2:e:183:GLY:C   | 3:e:1000:ADP:PA  | 2.98                     | 0.47              |
| 2:c:366:ARG:CG  | 3:b:1000:ADP:C4' | 2.89                     | 0.47              |
| 2:e:333:GLU:HA  | 2:e:336:LYS:CB   | 2.45                     | 0.47              |
| 2:e:352:LYS:CG  | 2:f:385:LYS:NZ   | 2.56                     | 0.47              |
| 2:c:213:PRO:HG3 | 2:c:231:THR:CG2  | 2.44                     | 0.47              |
| 2:c:305:ARG:NH2 | 2:b:213:PRO:CG   | 2.68                     | 0.47              |
| 2:a:80:TYR:N    | 2:a:111:PHE:O    | 2.45                     | 0.47              |
| 2:d:183:GLY:C   | 3:d:1000:ADP:PA  | 2.97                     | 0.47              |
| 1:8:1:DC:P      | 2:f:115:LYS:HZ1  | 2.37                     | 0.47              |
| 1:8:3:DC:C3'    | 1:8:3:DC:C2      | 2.98                     | 0.47              |
| 1:8:53:DC:C6    | 2:e:85:GLN:HG3   | 2.50                     | 0.47              |
| 1:8:58:DC:H5''  | 2:e:109:ARG:NH2  | 2.30                     | 0.47              |
| 2:e:280:ALA:CB  | 2:f:283:LYS:CD   | 2.83                     | 0.47              |
| 2:e:336:LYS:HD3 | 2:d:180:PRO:HG3  | 1.97                     | 0.47              |
| 2:f:184:LYS:CB  | 3:f:1000:ADP:PB  | 3.02                     | 0.47              |
| 2:c:183:GLY:C   | 3:c:1000:ADP:PA  | 2.97                     | 0.47              |
| 2:c:184:LYS:CB  | 3:c:1000:ADP:PB  | 3.03                     | 0.47              |
| 2:f:181:LYS:HD2 | 2:a:342:GLU:CD   | 2.39                     | 0.47              |
| 2:d:355:PHE:CE1 | 3:d:1000:ADP:C1' | 2.98                     | 0.47              |
| 2:e:184:LYS:N   | 3:e:1000:ADP:O3A | 2.43                     | 0.47              |
| 2:c:339:GLY:C   | 2:c:341:MET:H    | 2.23                     | 0.47              |
| 2:b:184:LYS:HG3 | 3:b:1000:ADP:PB  | 2.49                     | 0.47              |
| 2:d:184:LYS:CB  | 3:d:1000:ADP:PB  | 3.03                     | 0.46              |
| 1:8:58:DC:C5'   | 2:e:109:ARG:CZ   | 2.92                     | 0.46              |
| 2:f:184:LYS:CG  | 3:f:1000:ADP:PB  | 3.04                     | 0.46              |
| 2:c:338:THR:HA  | 2:b:212:ARG:HH22 | 1.80                     | 0.46              |
| 2:c:355:PHE:CE1 | 3:c:1000:ADP:C1' | 2.98                     | 0.46              |
| 2:e:80:TYR:N    | 2:e:111:PHE:O    | 2.45                     | 0.46              |
| 2:f:183:GLY:CA  | 3:f:1000:ADP:O5' | 2.56                     | 0.46              |
| 2:c:184:LYS:CG  | 3:c:1000:ADP:PB  | 3.03                     | 0.46              |
| 2:c:214:GLU:HA  | 2:d:138:PRO:CB   | 2.16                     | 0.46              |
| 2:b:183:GLY:C   | 3:b:1000:ADP:PA  | 2.98                     | 0.46              |
| 2:b:184:LYS:CG  | 3:b:1000:ADP:PB  | 3.04                     | 0.46              |
| 2:d:184:LYS:CG  | 3:d:1000:ADP:PB  | 3.04                     | 0.46              |
| 1:8:55:DC:C2    | 2:e:80:TYR:CE1   | 3.03                     | 0.46              |
| 2:e:355:PHE:CE1 | 3:e:1000:ADP:C1' | 2.98                     | 0.46              |
| 2:f:321:ILE:O   | 2:f:322:ASP:HB2  | 2.16                     | 0.46              |
| 2:c:183:GLY:HA2 | 3:c:1000:ADP:C8  | 2.35                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:b:184:LYS:CB    | 3:b:1000:ADP:PB   | 3.03                     | 0.46              |
| 2:b:366:ARG:CD    | 3:a:1000:ADP:H5'1 | 2.40                     | 0.46              |
| 2:e:184:LYS:CB    | 3:e:1000:ADP:PB   | 3.02                     | 0.46              |
| 2:b:333:GLU:O     | 2:b:334:GLU:C     | 2.57                     | 0.46              |
| 2:e:366:ARG:CZ    | 3:d:1000:ADP:H5'1 | 2.46                     | 0.46              |
| 2:b:302:GLY:CA    | 2:a:232:PHE:CZ    | 2.98                     | 0.46              |
| 2:e:280:ALA:HB2   | 2:f:283:LYS:HE2   | 1.98                     | 0.46              |
| 2:e:283:LYS:HD3   | 2:d:280:ALA:HB1   | 1.98                     | 0.46              |
| 2:e:333:GLU:O     | 2:e:336:LYS:N     | 2.47                     | 0.46              |
| 2:f:214:GLU:HB3   | 2:a:138:PRO:HB3   | 1.96                     | 0.46              |
| 2:c:352:LYS:HG2   | 2:d:385:LYS:HZ3   | 1.71                     | 0.46              |
| 1:8:11:DC:N1      | 2:a:88:ARG:CZ     | 2.75                     | 0.46              |
| 2:c:324:GLY:HA3   | 2:d:333:GLU:CB    | 2.46                     | 0.46              |
| 2:b:183:GLY:HA2   | 3:b:1000:ADP:C8   | 2.35                     | 0.46              |
| 2:a:183:GLY:C     | 3:a:1000:ADP:PA   | 2.98                     | 0.46              |
| 1:8:58:DC:O5'     | 2:e:109:ARG:NH1   | 2.49                     | 0.45              |
| 2:f:184:LYS:CD    | 3:f:1000:ADP:O3B  | 2.61                     | 0.45              |
| 2:f:324:GLY:N     | 2:a:333:GLU:HB3   | 2.30                     | 0.45              |
| 2:a:355:PHE:CE1   | 3:a:1000:ADP:C1'  | 2.98                     | 0.45              |
| 2:e:366:ARG:CG    | 3:d:1000:ADP:C4'  | 2.92                     | 0.45              |
| 2:f:353:ARG:HH21  | 2:a:364:GLY:HA3   | 1.79                     | 0.45              |
| 1:8:53:DC:O2      | 1:8:53:DC:H5''    | 2.17                     | 0.45              |
| 2:f:67:SER:OG     | 2:f:69:ASP:OD1    | 2.32                     | 0.45              |
| 2:f:325:SER:C     | 2:f:327:MET:H     | 2.24                     | 0.45              |
| 2:c:80:TYR:N      | 2:c:111:PHE:O     | 2.45                     | 0.45              |
| 1:8:54:DC:C6      | 1:8:54:DC:C4'     | 3.00                     | 0.45              |
| 2:e:212:ARG:HA    | 2:e:232:PHE:CE2   | 2.51                     | 0.45              |
| 3:e:1000:ADP:C4'  | 2:f:366:ARG:HD3   | 2.44                     | 0.45              |
| 2:d:147:MET:HE1   | 2:d:195:ILE:HG13  | 1.99                     | 0.45              |
| 2:d:328:ASP:O     | 2:d:332:TYR:N     | 2.45                     | 0.45              |
| 1:8:4:DC:C6       | 1:8:4:DC:C4'      | 3.00                     | 0.45              |
| 2:f:147:MET:HE1   | 2:f:195:ILE:HG13  | 1.99                     | 0.45              |
| 2:c:147:MET:HE1   | 2:c:195:ILE:HG13  | 1.99                     | 0.45              |
| 2:b:332:TYR:CG    | 2:b:333:GLU:N     | 2.84                     | 0.45              |
| 3:c:1000:ADP:O2A  | 2:d:366:ARG:NH2   | 2.49                     | 0.45              |
| 2:a:66:ARG:NH1    | 2:a:78:ASP:OD2    | 2.50                     | 0.45              |
| 2:d:183:GLY:N     | 3:d:1000:ADP:O3A  | 2.41                     | 0.45              |
| 1:8:1:DC:H5''     | 2:f:115:LYS:CG    | 2.29                     | 0.45              |
| 1:8:44:DC:C6      | 1:8:44:DC:C4'     | 3.00                     | 0.45              |
| 3:e:1000:ADP:H5'1 | 2:f:366:ARG:CZ    | 2.47                     | 0.45              |
| 2:f:66:ARG:NH1    | 2:f:78:ASP:OD2    | 2.50                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:c:66:ARG:NH1   | 2:c:78:ASP:OD2   | 2.50                     | 0.45              |
| 2:b:302:GLY:HA3  | 2:a:232:PHE:CE1  | 2.52                     | 0.45              |
| 2:a:147:MET:HE1  | 2:a:195:ILE:HG13 | 1.99                     | 0.45              |
| 2:d:66:ARG:NH1   | 2:d:78:ASP:OD2   | 2.50                     | 0.45              |
| 1:8:33:DC:N3     | 2:c:84:SER:OG    | 2.47                     | 0.45              |
| 2:f:355:PHE:CE1  | 3:f:1000:ADP:C1' | 2.98                     | 0.45              |
| 2:b:305:ARG:NH1  | 2:a:213:PRO:HG2  | 2.28                     | 0.45              |
| 2:a:184:LYS:CD   | 3:a:1000:ADP:O3B | 2.62                     | 0.45              |
| 1:8:4:DC:C6      | 1:8:4:DC:C5'     | 2.86                     | 0.45              |
| 2:a:184:LYS:CB   | 3:a:1000:ADP:PB  | 3.03                     | 0.45              |
| 2:b:333:GLU:HB3  | 2:a:324:GLY:CA   | 2.47                     | 0.44              |
| 1:8:38:DC:O2     | 1:8:38:DC:H2''   | 2.17                     | 0.44              |
| 2:e:333:GLU:C    | 2:d:323:THR:O    | 2.59                     | 0.44              |
| 2:c:208:LEU:HB3  | 2:c:211:GLU:HG3  | 2.00                     | 0.44              |
| 2:d:80:TYR:N     | 2:d:111:PHE:O    | 2.45                     | 0.44              |
| 2:d:184:LYS:HG3  | 3:d:1000:ADP:PB  | 2.49                     | 0.44              |
| 2:e:184:LYS:CG   | 3:e:1000:ADP:PB  | 3.03                     | 0.44              |
| 3:f:1000:ADP:O1B | 2:a:366:ARG:NH2  | 2.40                     | 0.44              |
| 2:c:333:GLU:HB3  | 2:b:323:THR:O    | 2.17                     | 0.44              |
| 2:c:366:ARG:NH2  | 3:b:1000:ADP:O2B | 2.43                     | 0.44              |
| 2:b:355:PHE:CZ   | 3:b:1000:ADP:C1' | 3.00                     | 0.44              |
| 2:a:184:LYS:CG   | 3:a:1000:ADP:PB  | 3.04                     | 0.44              |
| 2:d:355:PHE:CZ   | 3:d:1000:ADP:C1' | 3.00                     | 0.44              |
| 2:e:276:THR:HG23 | 2:f:292:ASN:OD1  | 2.17                     | 0.44              |
| 2:f:79:ILE:HG12  | 2:f:101:ILE:HG21 | 2.00                     | 0.44              |
| 2:f:331:ILE:O    | 2:f:332:TYR:C    | 2.61                     | 0.44              |
| 2:c:79:ILE:HG12  | 2:c:101:ILE:HG21 | 2.00                     | 0.44              |
| 2:c:326:LYS:HE2  | 2:d:286:THR:HB   | 1.94                     | 0.44              |
| 2:e:79:ILE:HG12  | 2:e:101:ILE:HG21 | 2.00                     | 0.44              |
| 2:e:330:VAL:O    | 2:e:334:GLU:HB3  | 2.17                     | 0.44              |
| 2:e:332:TYR:CE2  | 2:e:333:GLU:HG3  | 2.53                     | 0.44              |
| 2:f:217:THR:CG2  | 2:a:138:PRO:O    | 2.65                     | 0.44              |
| 2:c:330:VAL:O    | 2:c:334:GLU:HB3  | 2.16                     | 0.44              |
| 2:c:355:PHE:CZ   | 3:c:1000:ADP:C1' | 3.00                     | 0.44              |
| 2:b:184:LYS:CD   | 3:b:1000:ADP:O3B | 2.61                     | 0.44              |
| 2:f:183:GLY:HA2  | 3:f:1000:ADP:C8  | 2.35                     | 0.44              |
| 2:f:387:ILE:HG23 | 2:f:395:ALA:HB1  | 1.99                     | 0.44              |
| 2:c:342:GLU:OE1  | 2:b:181:LYS:CD   | 2.64                     | 0.44              |
| 2:b:147:MET:HE1  | 2:b:195:ILE:HG13 | 1.99                     | 0.44              |
| 2:e:387:ILE:HG23 | 2:e:395:ALA:HB1  | 1.99                     | 0.44              |
| 2:c:286:THR:HG22 | 2:b:326:LYS:HZ2  | 1.74                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:a:297:PRO:HB2  | 2:a:335:PHE:HZ   | 1.83                     | 0.44              |
| 2:a:387:ILE:HG23 | 2:a:395:ALA:HB1  | 1.99                     | 0.44              |
| 1:8:11:DC:C2'    | 2:a:88:ARG:HD2   | 2.48                     | 0.44              |
| 2:e:66:ARG:NH1   | 2:e:78:ASP:OD2   | 2.50                     | 0.44              |
| 2:f:321:ILE:HG22 | 2:f:332:TYR:CD2  | 2.52                     | 0.44              |
| 2:c:333:GLU:O    | 2:c:334:GLU:C    | 2.61                     | 0.44              |
| 2:b:66:ARG:NH1   | 2:b:78:ASP:OD2   | 2.50                     | 0.44              |
| 1:8:24:DC:H6     | 1:8:24:DC:C5'    | 2.30                     | 0.43              |
| 1:8:44:DC:C6     | 1:8:44:DC:C5'    | 2.86                     | 0.43              |
| 2:e:67:SER:OG    | 2:e:69:ASP:OD1   | 2.32                     | 0.43              |
| 2:f:297:PRO:HB2  | 2:f:335:PHE:HZ   | 1.83                     | 0.43              |
| 2:c:276:THR:CG2  | 2:d:292:ASN:OD1  | 2.62                     | 0.43              |
| 2:e:333:GLU:O    | 2:e:334:GLU:C    | 2.61                     | 0.43              |
| 2:d:297:PRO:HB2  | 2:d:335:PHE:HZ   | 1.84                     | 0.43              |
| 1:8:40:DC:N3     | 2:d:87:ARG:O     | 2.51                     | 0.43              |
| 2:e:138:PRO:CG   | 2:d:213:PRO:C    | 2.83                     | 0.43              |
| 2:e:147:MET:HE1  | 2:e:195:ILE:HG13 | 1.99                     | 0.43              |
| 2:f:180:PRO:CB   | 2:a:337:GLY:HA2  | 2.47                     | 0.43              |
| 2:c:387:ILE:HG23 | 2:c:395:ALA:HB1  | 1.99                     | 0.43              |
| 2:c:138:PRO:HB2  | 2:b:214:GLU:HB3  | 1.95                     | 0.43              |
| 2:c:366:ARG:CZ   | 3:b:1000:ADP:C5' | 2.96                     | 0.43              |
| 2:a:355:PHE:CZ   | 3:a:1000:ADP:C1' | 3.00                     | 0.43              |
| 2:d:79:ILE:HG12  | 2:d:101:ILE:HG21 | 2.00                     | 0.43              |
| 1:8:41:DC:O3'    | 2:d:88:ARG:NH1   | 2.52                     | 0.43              |
| 2:c:212:ARG:NH2  | 2:d:173:ARG:NH2  | 2.67                     | 0.43              |
| 2:c:214:GLU:N    | 2:d:138:PRO:CG   | 2.81                     | 0.43              |
| 2:a:184:LYS:HG3  | 3:a:1000:ADP:PB  | 2.49                     | 0.43              |
| 2:d:387:ILE:HG23 | 2:d:395:ALA:HB1  | 1.99                     | 0.43              |
| 2:b:79:ILE:HG12  | 2:b:101:ILE:HG21 | 2.00                     | 0.43              |
| 2:e:138:PRO:HG2  | 2:d:214:GLU:N    | 2.33                     | 0.43              |
| 2:e:272:ARG:NH2  | 2:f:334:GLU:OE1  | 2.50                     | 0.43              |
| 1:8:11:DC:C6     | 1:8:11:DC:C3'    | 3.02                     | 0.43              |
| 2:f:80:TYR:N     | 2:f:111:PHE:O    | 2.45                     | 0.43              |
| 2:f:355:PHE:CZ   | 3:f:1000:ADP:C1' | 3.00                     | 0.43              |
| 2:b:387:ILE:HG23 | 2:b:395:ALA:HB1  | 1.99                     | 0.43              |
| 2:e:297:PRO:HB2  | 2:e:335:PHE:HZ   | 1.84                     | 0.43              |
| 2:f:296:ARG:HB2  | 2:f:297:PRO:HD3  | 2.01                     | 0.43              |
| 2:c:213:PRO:O    | 2:c:216:VAL:N    | 2.51                     | 0.43              |
| 2:c:305:ARG:HH22 | 2:b:213:PRO:HG2  | 1.73                     | 0.43              |
| 2:a:67:SER:OG    | 2:a:69:ASP:OD1   | 2.31                     | 0.43              |
| 1:8:31:DC:C6     | 1:8:31:DC:C3'    | 3.02                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:e:301:PHE:HE2   | 2:e:338:THR:O    | 2.01                     | 0.43              |
| 2:e:355:PHE:CZ    | 3:e:1000:ADP:C1' | 3.00                     | 0.43              |
| 2:b:138:PRO:O     | 2:a:217:THR:CG2  | 2.65                     | 0.43              |
| 1:8:14:DC:H6      | 1:8:14:DC:C5'    | 2.31                     | 0.42              |
| 2:e:213:PRO:O     | 2:e:214:GLU:C    | 2.62                     | 0.42              |
| 2:f:232:PHE:CZ    | 2:a:302:GLY:HA3  | 2.54                     | 0.42              |
| 3:c:1000:ADP:O3'  | 2:d:366:ARG:CB   | 2.42                     | 0.42              |
| 3:c:1000:ADP:HO3' | 2:d:366:ARG:HB3  | 1.74                     | 0.42              |
| 2:b:366:ARG:NE    | 3:a:1000:ADP:C5' | 2.76                     | 0.42              |
| 1:8:41:DC:C4'     | 2:d:88:ARG:HH11  | 2.32                     | 0.42              |
| 2:c:366:ARG:NH1   | 2:b:181:LYS:H    | 1.77                     | 0.42              |
| 2:c:297:PRO:HB2   | 2:c:335:PHE:HZ   | 1.83                     | 0.42              |
| 2:d:321:ILE:HG22  | 2:d:332:TYR:CE2  | 2.53                     | 0.42              |
| 2:e:184:LYS:CD    | 3:e:1000:ADP:O3B | 2.61                     | 0.42              |
| 2:a:79:ILE:HG12   | 2:a:101:ILE:HG21 | 2.00                     | 0.42              |
| 1:8:14:DC:N4      | 2:a:102:ARG:HH21 | 2.14                     | 0.42              |
| 2:e:138:PRO:O     | 2:d:217:THR:CG2  | 2.67                     | 0.42              |
| 2:e:296:ARG:HB2   | 2:e:297:PRO:HD3  | 2.01                     | 0.42              |
| 2:e:333:GLU:O     | 2:e:336:LYS:HB3  | 2.20                     | 0.42              |
| 2:d:296:ARG:HB2   | 2:d:297:PRO:HD3  | 2.01                     | 0.42              |
| 1:8:21:DC:C2'     | 2:b:88:ARG:HD2   | 2.46                     | 0.42              |
| 2:b:366:ARG:CD    | 3:a:1000:ADP:C4' | 2.96                     | 0.42              |
| 1:8:3:DC:H3'      | 1:8:3:DC:C2      | 2.51                     | 0.42              |
| 2:d:67:SER:OG     | 2:d:69:ASP:OD1   | 2.32                     | 0.42              |
| 2:d:332:TYR:CG    | 2:d:333:GLU:N    | 2.86                     | 0.42              |
| 2:f:272:ARG:NH2   | 2:a:334:GLU:CD   | 2.73                     | 0.42              |
| 1:8:55:DC:O2      | 2:e:80:TYR:CZ    | 2.73                     | 0.42              |
| 2:a:176:ILE:HB    | 2:a:318:THR:HG22 | 2.01                     | 0.42              |
| 2:b:176:ILE:HB    | 2:b:318:THR:HG22 | 2.01                     | 0.41              |
| 1:8:43:DC:O2      | 1:8:43:DC:H3'    | 2.20                     | 0.41              |
| 2:b:296:ARG:HB2   | 2:b:297:PRO:HD3  | 2.01                     | 0.41              |
| 2:e:176:ILE:HB    | 2:e:318:THR:HG22 | 2.02                     | 0.41              |
| 2:e:339:GLY:H     | 2:d:212:ARG:HH22 | 1.69                     | 0.41              |
| 1:8:13:DC:N4      | 2:a:113:LEU:O    | 2.53                     | 0.41              |
| 1:8:34:DC:H6      | 1:8:34:DC:O5'    | 2.02                     | 0.41              |
| 2:e:334:GLU:HG3   | 2:e:335:PHE:N    | 2.36                     | 0.41              |
| 2:f:176:ILE:HB    | 2:f:318:THR:HG22 | 2.02                     | 0.41              |
| 2:c:176:ILE:HB    | 2:c:318:THR:HG22 | 2.01                     | 0.41              |
| 2:c:324:GLY:HA3   | 2:d:333:GLU:HB3  | 2.02                     | 0.41              |
| 2:d:327:MET:O     | 2:d:331:ILE:N    | 2.41                     | 0.41              |
| 2:e:184:LYS:C     | 3:e:1000:ADP:O2A | 2.60                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:c:324:GLY:HA3   | 2:d:333:GLU:CD   | 2.46                     | 0.41              |
| 3:c:1000:ADP:H5'1 | 2:d:366:ARG:NE   | 2.36                     | 0.41              |
| 2:a:183:GLY:CA    | 3:a:1000:ADP:O5' | 2.56                     | 0.41              |
| 1:8:33:DC:H42     | 2:c:85:GLN:CD    | 2.21                     | 0.41              |
| 2:c:183:GLY:CA    | 3:c:1000:ADP:O1A | 2.69                     | 0.41              |
| 1:8:11:DC:C6      | 2:a:88:ARG:NH2   | 2.88                     | 0.41              |
| 1:8:56:DC:N4      | 2:e:110:TYR:HD2  | 2.17                     | 0.41              |
| 2:e:213:PRO:HG2   | 2:f:305:ARG:HH22 | 1.83                     | 0.41              |
| 2:d:176:ILE:HB    | 2:d:318:THR:HG22 | 2.02                     | 0.41              |
| 2:f:212:ARG:HG2   | 2:f:215:GLU:CD   | 2.46                     | 0.41              |
| 2:c:264:LEU:HD22  | 2:c:300:PHE:HE1  | 1.86                     | 0.41              |
| 2:c:296:ARG:HB2   | 2:c:297:PRO:HD3  | 2.01                     | 0.41              |
| 2:e:138:PRO:CG    | 2:d:213:PRO:CB   | 2.64                     | 0.41              |
| 2:e:183:GLY:CA    | 3:e:1000:ADP:O2A | 2.68                     | 0.41              |
| 2:f:213:PRO:O     | 2:f:214:GLU:C    | 2.64                     | 0.41              |
| 2:c:183:GLY:N     | 3:c:1000:ADP:O3A | 2.41                     | 0.41              |
| 2:c:184:LYS:CD    | 3:c:1000:ADP:O1B | 2.61                     | 0.41              |
| 2:c:366:ARG:CD    | 3:b:1000:ADP:H4' | 2.50                     | 0.41              |
| 2:b:138:PRO:HB3   | 2:a:214:GLU:HB3  | 2.02                     | 0.41              |
| 2:b:148:GLU:O     | 2:b:198:ASN:ND2  | 2.54                     | 0.41              |
| 2:a:296:ARG:HB2   | 2:a:297:PRO:HD3  | 2.02                     | 0.41              |
| 2:d:148:GLU:O     | 2:d:198:ASN:ND2  | 2.54                     | 0.41              |
| 2:d:149:ARG:HH21  | 2:d:193:GLN:HB3  | 1.86                     | 0.41              |
| 2:f:212:ARG:NH1   | 2:a:338:THR:HG22 | 2.35                     | 0.41              |
| 2:b:283:LYS:CD    | 2:a:280:ALA:HB2  | 2.50                     | 0.41              |
| 1:8:11:DC:H2'     | 2:a:88:ARG:HD2   | 2.02                     | 0.40              |
| 2:a:264:LEU:HD22  | 2:a:300:PHE:HE1  | 1.86                     | 0.40              |
| 2:a:274:TYR:HA    | 2:a:277:VAL:HG22 | 2.03                     | 0.40              |
| 2:e:213:PRO:O     | 2:e:216:VAL:N    | 2.54                     | 0.40              |
| 2:f:213:PRO:HG3   | 2:f:231:THR:CG2  | 2.52                     | 0.40              |
| 2:b:274:TYR:HA    | 2:b:277:VAL:HG22 | 2.04                     | 0.40              |
| 2:f:181:LYS:NZ    | 2:a:342:GLU:OE1  | 2.51                     | 0.40              |
| 2:f:183:GLY:CA    | 3:f:1000:ADP:O2A | 2.68                     | 0.40              |
| 2:f:264:LEU:HD22  | 2:f:300:PHE:HE1  | 1.86                     | 0.40              |
| 3:f:1000:ADP:HO3' | 2:a:366:ARG:CB   | 2.06                     | 0.40              |
| 2:d:184:LYS:CD    | 3:d:1000:ADP:O1B | 2.62                     | 0.40              |
| 1:8:53:DC:O2      | 1:8:53:DC:H3'    | 2.21                     | 0.40              |
| 2:e:349:ILE:HG12  | 2:e:393:ILE:HG12 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

### 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 |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 2   | a     | 357/359 (99%)   | 355 (99%)  | 2 (1%)   | 78          | 80 |
| 2   | b     | 357/359 (99%)   | 353 (99%)  | 4 (1%)   | 65          | 74 |
| 2   | c     | 357/359 (99%)   | 349 (98%)  | 8 (2%)   | 45          | 64 |
| 2   | d     | 357/359 (99%)   | 351 (98%)  | 6 (2%)   | 53          | 68 |
| 2   | e     | 357/359 (99%)   | 349 (98%)  | 8 (2%)   | 45          | 64 |
| 2   | f     | 357/359 (99%)   | 350 (98%)  | 7 (2%)   | 48          | 66 |
| All | All   | 2142/2154 (99%) | 2107 (98%) | 35 (2%)  | 54          | 69 |

All (35) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | e     | 3   | LEU  |
| 2   | e     | 188 | LEU  |
| 2   | e     | 211 | GLU  |
| 2   | e     | 212 | ARG  |
| 2   | e     | 332 | TYR  |
| 2   | e     | 334 | GLU  |
| 2   | e     | 336 | LYS  |
| 2   | e     | 338 | THR  |
| 2   | f     | 3   | LEU  |
| 2   | f     | 188 | LEU  |
| 2   | f     | 211 | GLU  |
| 2   | f     | 212 | ARG  |
| 2   | f     | 323 | THR  |
| 2   | f     | 325 | SER  |
| 2   | f     | 332 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | c     | 3   | LEU  |
| 2   | c     | 188 | LEU  |
| 2   | c     | 211 | GLU  |
| 2   | c     | 212 | ARG  |
| 2   | c     | 332 | TYR  |
| 2   | c     | 334 | GLU  |
| 2   | c     | 338 | THR  |
| 2   | c     | 340 | ASN  |
| 2   | b     | 3   | LEU  |
| 2   | b     | 188 | LEU  |
| 2   | b     | 332 | TYR  |
| 2   | b     | 334 | GLU  |
| 2   | a     | 3   | LEU  |
| 2   | a     | 188 | LEU  |
| 2   | d     | 3   | LEU  |
| 2   | d     | 188 | LEU  |
| 2   | d     | 331 | ILE  |
| 2   | d     | 332 | TYR  |
| 2   | d     | 333 | GLU  |
| 2   | d     | 334 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | e     | 85  | GLN  |
| 2   | e     | 241 | GLN  |
| 2   | e     | 256 | HIS  |
| 2   | f     | 241 | GLN  |
| 2   | f     | 256 | HIS  |
| 2   | c     | 85  | GLN  |
| 2   | c     | 172 | GLN  |
| 2   | c     | 241 | GLN  |
| 2   | c     | 256 | HIS  |
| 2   | b     | 241 | GLN  |
| 2   | b     | 256 | HIS  |
| 2   | a     | 241 | GLN  |
| 2   | a     | 256 | HIS  |
| 2   | d     | 241 | GLN  |
| 2   | d     | 256 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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$ |
| 5   | BEF  | a     | 1002 | 3,2  | 0,3,3        | -    | -           | -           |      |             |
| 5   | BEF  | c     | 1002 | 3,2  | 0,3,3        | -    | -           | -           |      |             |
| 5   | BEF  | d     | 1002 | 3,2  | 0,3,3        | -    | -           | -           |      |             |
| 3   | ADP  | e     | 1000 | 4,5  | 28,29,29     | 1.43 | 5 (17%)     | 43,45,45    | 1.87 | 12 (27%)    |
| 5   | BEF  | e     | 1002 | 3,2  | 0,3,3        | -    | -           | -           |      |             |
| 5   | BEF  | f     | 1002 | 3,2  | 0,3,3        | -    | -           | -           |      |             |
| 3   | ADP  | a     | 1000 | 4,5  | 28,29,29     | 1.42 | 5 (17%)     | 43,45,45    | 1.86 | 13 (30%)    |
| 3   | ADP  | c     | 1000 | 4,5  | 28,29,29     | 1.42 | 5 (17%)     | 43,45,45    | 1.86 | 12 (27%)    |
| 3   | ADP  | f     | 1000 | 4,5  | 28,29,29     | 1.43 | 5 (17%)     | 43,45,45    | 1.86 | 12 (27%)    |
| 3   | ADP  | d     | 1000 | 4,5  | 28,29,29     | 1.43 | 5 (17%)     | 43,45,45    | 1.87 | 12 (27%)    |
| 3   | ADP  | b     | 1000 | 4,5  | 28,29,29     | 1.42 | 5 (17%)     | 43,45,45    | 1.86 | 13 (30%)    |
| 5   | BEF  | b     | 1002 | 3,2  | 0,3,3        | -    | -           | -           |      |             |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | ADP  | e     | 1000 | 4,5  | -       | 0/16/32/32 | 0/3/3/3 |
| 3   | ADP  | a     | 1000 | 4,5  | -       | 0/16/32/32 | 0/3/3/3 |
| 3   | ADP  | c     | 1000 | 4,5  | -       | 0/16/32/32 | 0/3/3/3 |
| 3   | ADP  | f     | 1000 | 4,5  | -       | 0/16/32/32 | 0/3/3/3 |
| 3   | ADP  | d     | 1000 | 4,5  | -       | 0/16/32/32 | 0/3/3/3 |
| 3   | ADP  | b     | 1000 | 4,5  | -       | 0/16/32/32 | 0/3/3/3 |

All (30) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 3   | d     | 1000 | ADP  | C5-C4  | 4.75  | 1.47        | 1.39     |
| 3   | f     | 1000 | ADP  | C5-C4  | 4.71  | 1.47        | 1.39     |
| 3   | e     | 1000 | ADP  | C5-C4  | 4.69  | 1.47        | 1.39     |
| 3   | c     | 1000 | ADP  | C5-C4  | 4.67  | 1.47        | 1.39     |
| 3   | b     | 1000 | ADP  | C5-C4  | 4.67  | 1.47        | 1.39     |
| 3   | a     | 1000 | ADP  | C5-C4  | 4.63  | 1.47        | 1.39     |
| 3   | a     | 1000 | ADP  | C5-C6  | 2.85  | 1.48        | 1.41     |
| 3   | b     | 1000 | ADP  | C5-C6  | 2.82  | 1.48        | 1.41     |
| 3   | d     | 1000 | ADP  | C5-C6  | 2.81  | 1.48        | 1.41     |
| 3   | e     | 1000 | ADP  | C5-C6  | 2.79  | 1.48        | 1.41     |
| 3   | f     | 1000 | ADP  | C5-C6  | 2.78  | 1.48        | 1.41     |
| 3   | c     | 1000 | ADP  | C5-C6  | 2.76  | 1.48        | 1.41     |
| 3   | e     | 1000 | ADP  | PA-O3A | 2.41  | 1.62        | 1.59     |
| 3   | a     | 1000 | ADP  | PA-O3A | 2.39  | 1.62        | 1.59     |
| 3   | b     | 1000 | ADP  | C8-N7  | 2.34  | 1.36        | 1.31     |
| 3   | c     | 1000 | ADP  | C8-N7  | 2.27  | 1.36        | 1.31     |
| 3   | c     | 1000 | ADP  | PA-O3A | 2.24  | 1.61        | 1.59     |
| 3   | f     | 1000 | ADP  | PA-O3A | 2.21  | 1.61        | 1.59     |
| 3   | a     | 1000 | ADP  | C8-N7  | 2.19  | 1.35        | 1.31     |
| 3   | d     | 1000 | ADP  | PA-O3A | 2.19  | 1.61        | 1.59     |
| 3   | f     | 1000 | ADP  | C8-N7  | 2.17  | 1.35        | 1.31     |
| 3   | d     | 1000 | ADP  | C8-N7  | 2.15  | 1.35        | 1.31     |
| 3   | d     | 1000 | ADP  | C5-N7  | -2.13 | 1.35        | 1.39     |
| 3   | e     | 1000 | ADP  | C8-N7  | 2.11  | 1.35        | 1.31     |
| 3   | b     | 1000 | ADP  | PA-O3A | 2.10  | 1.61        | 1.59     |
| 3   | a     | 1000 | ADP  | C5-N7  | -2.10 | 1.35        | 1.39     |
| 3   | b     | 1000 | ADP  | C5-N7  | -2.09 | 1.35        | 1.39     |
| 3   | e     | 1000 | ADP  | C5-N7  | -2.04 | 1.35        | 1.39     |
| 3   | c     | 1000 | ADP  | C5-N7  | -2.02 | 1.35        | 1.39     |
| 3   | f     | 1000 | ADP  | C5-N7  | -2.00 | 1.35        | 1.39     |

All (74) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | e     | 1000 | ADP  | C5-C4-N3   | -5.50 | 119.14      | 126.72   |
| 3   | c     | 1000 | ADP  | C5-C4-N3   | -5.48 | 119.18      | 126.72   |
| 3   | f     | 1000 | ADP  | C5-C4-N3   | -5.46 | 119.20      | 126.72   |
| 3   | d     | 1000 | ADP  | C5-C4-N3   | -5.42 | 119.26      | 126.72   |
| 3   | b     | 1000 | ADP  | C5-C4-N3   | -5.38 | 119.31      | 126.72   |
| 3   | a     | 1000 | ADP  | C5-C4-N3   | -5.33 | 119.38      | 126.72   |
| 3   | c     | 1000 | ADP  | N3-C4-N9   | 4.39  | 134.63      | 127.17   |
| 3   | d     | 1000 | ADP  | N3-C4-N9   | 4.38  | 134.61      | 127.17   |
| 3   | e     | 1000 | ADP  | N3-C4-N9   | 4.37  | 134.60      | 127.17   |
| 3   | b     | 1000 | ADP  | N3-C4-N9   | 4.36  | 134.59      | 127.17   |
| 3   | f     | 1000 | ADP  | N3-C4-N9   | 4.36  | 134.58      | 127.17   |
| 3   | a     | 1000 | ADP  | N3-C4-N9   | 4.33  | 134.53      | 127.17   |
| 3   | f     | 1000 | ADP  | C4-C5-N7   | -3.78 | 106.26      | 110.58   |
| 3   | e     | 1000 | ADP  | C4-C5-N7   | -3.77 | 106.27      | 110.58   |
| 3   | d     | 1000 | ADP  | C4-C5-N7   | -3.69 | 106.37      | 110.58   |
| 3   | e     | 1000 | ADP  | C2-N3-C4   | 3.63  | 120.70      | 111.83   |
| 3   | c     | 1000 | ADP  | C4-C5-N7   | -3.63 | 106.43      | 110.58   |
| 3   | f     | 1000 | ADP  | C2-N3-C4   | 3.62  | 120.67      | 111.83   |
| 3   | b     | 1000 | ADP  | C4-C5-N7   | -3.62 | 106.45      | 110.58   |
| 3   | d     | 1000 | ADP  | C2-N3-C4   | 3.61  | 120.66      | 111.83   |
| 3   | a     | 1000 | ADP  | C2-N3-C4   | 3.61  | 120.65      | 111.83   |
| 3   | b     | 1000 | ADP  | C2-N3-C4   | 3.60  | 120.62      | 111.83   |
| 3   | a     | 1000 | ADP  | C4-C5-N7   | -3.59 | 106.47      | 110.58   |
| 3   | c     | 1000 | ADP  | C2-N3-C4   | 3.59  | 120.60      | 111.83   |
| 3   | d     | 1000 | ADP  | N3-C2-N1   | -3.43 | 123.40      | 128.58   |
| 3   | e     | 1000 | ADP  | N3-C2-N1   | -3.42 | 123.41      | 128.58   |
| 3   | a     | 1000 | ADP  | N3-C2-N1   | -3.38 | 123.47      | 128.58   |
| 3   | f     | 1000 | ADP  | N3-C2-N1   | -3.36 | 123.49      | 128.58   |
| 3   | c     | 1000 | ADP  | N3-C2-N1   | -3.35 | 123.51      | 128.58   |
| 3   | b     | 1000 | ADP  | N3-C2-N1   | -3.35 | 123.51      | 128.58   |
| 3   | b     | 1000 | ADP  | C4-N9-C8   | 3.15  | 109.05      | 105.74   |
| 3   | a     | 1000 | ADP  | C4-N9-C8   | 3.12  | 109.02      | 105.74   |
| 3   | f     | 1000 | ADP  | C4-N9-C8   | 3.09  | 108.98      | 105.74   |
| 3   | d     | 1000 | ADP  | C4-N9-C8   | 3.07  | 108.96      | 105.74   |
| 3   | c     | 1000 | ADP  | C4-N9-C8   | 3.05  | 108.94      | 105.74   |
| 3   | e     | 1000 | ADP  | C4-N9-C8   | 2.94  | 108.82      | 105.74   |
| 3   | a     | 1000 | ADP  | C5-N7-C8   | 2.81  | 107.87      | 103.45   |
| 3   | b     | 1000 | ADP  | C2'-C1'-N9 | -2.79 | 106.38      | 113.30   |
| 3   | d     | 1000 | ADP  | C5-N7-C8   | 2.78  | 107.82      | 103.45   |
| 3   | f     | 1000 | ADP  | C5-N7-C8   | 2.78  | 107.82      | 103.45   |
| 3   | d     | 1000 | ADP  | C2'-C1'-N9 | -2.77 | 106.41      | 113.30   |
| 3   | e     | 1000 | ADP  | C2'-C1'-N9 | -2.77 | 106.42      | 113.30   |
| 3   | e     | 1000 | ADP  | C5-N7-C8   | 2.76  | 107.79      | 103.45   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | b     | 1000 | ADP  | C5-N7-C8   | 2.75  | 107.78      | 103.45   |
| 3   | c     | 1000 | ADP  | C2'-C1'-N9 | -2.74 | 106.50      | 113.30   |
| 3   | a     | 1000 | ADP  | C2'-C1'-N9 | -2.73 | 106.53      | 113.30   |
| 3   | c     | 1000 | ADP  | C5-N7-C8   | 2.72  | 107.72      | 103.45   |
| 3   | f     | 1000 | ADP  | C2'-C1'-N9 | -2.70 | 106.59      | 113.30   |
| 3   | f     | 1000 | ADP  | C6-C5-N7   | 2.40  | 136.71      | 132.09   |
| 3   | d     | 1000 | ADP  | C6-C5-N7   | 2.39  | 136.70      | 132.09   |
| 3   | e     | 1000 | ADP  | C6-C5-N7   | 2.39  | 136.69      | 132.09   |
| 3   | a     | 1000 | ADP  | N9-C8-N7   | -2.38 | 110.56      | 113.94   |
| 3   | a     | 1000 | ADP  | C6-C5-N7   | 2.38  | 136.67      | 132.09   |
| 3   | b     | 1000 | ADP  | N9-C8-N7   | -2.34 | 110.62      | 113.94   |
| 3   | b     | 1000 | ADP  | C6-C5-N7   | 2.34  | 136.60      | 132.09   |
| 3   | c     | 1000 | ADP  | C6-C5-N7   | 2.31  | 136.54      | 132.09   |
| 3   | c     | 1000 | ADP  | N9-C8-N7   | -2.28 | 110.71      | 113.94   |
| 3   | d     | 1000 | ADP  | N9-C8-N7   | -2.27 | 110.72      | 113.94   |
| 3   | f     | 1000 | ADP  | N9-C8-N7   | -2.27 | 110.72      | 113.94   |
| 3   | e     | 1000 | ADP  | N9-C8-N7   | -2.17 | 110.85      | 113.94   |
| 3   | e     | 1000 | ADP  | C2-N1-C6   | 2.16  | 122.27      | 118.73   |
| 3   | d     | 1000 | ADP  | C2-N1-C6   | 2.14  | 122.25      | 118.73   |
| 3   | e     | 1000 | ADP  | O2A-PA-O1A | 2.13  | 122.35      | 112.44   |
| 3   | d     | 1000 | ADP  | O2A-PA-O1A | 2.13  | 122.35      | 112.44   |
| 3   | f     | 1000 | ADP  | O2A-PA-O1A | 2.12  | 122.33      | 112.44   |
| 3   | b     | 1000 | ADP  | C2-N1-C6   | 2.11  | 122.19      | 118.73   |
| 3   | c     | 1000 | ADP  | O2A-PA-O1A | 2.10  | 122.23      | 112.44   |
| 3   | a     | 1000 | ADP  | O2A-PA-O1A | 2.10  | 122.20      | 112.44   |
| 3   | b     | 1000 | ADP  | O2A-PA-O1A | 2.09  | 122.18      | 112.44   |
| 3   | c     | 1000 | ADP  | C2-N1-C6   | 2.08  | 122.14      | 118.73   |
| 3   | f     | 1000 | ADP  | C2-N1-C6   | 2.08  | 122.14      | 118.73   |
| 3   | a     | 1000 | ADP  | C2-N1-C6   | 2.06  | 122.11      | 118.73   |
| 3   | b     | 1000 | ADP  | O3B-PB-O2B | 2.02  | 115.39      | 107.80   |
| 3   | a     | 1000 | ADP  | O3B-PB-O2B | 2.02  | 115.38      | 107.80   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 362 short contacts:

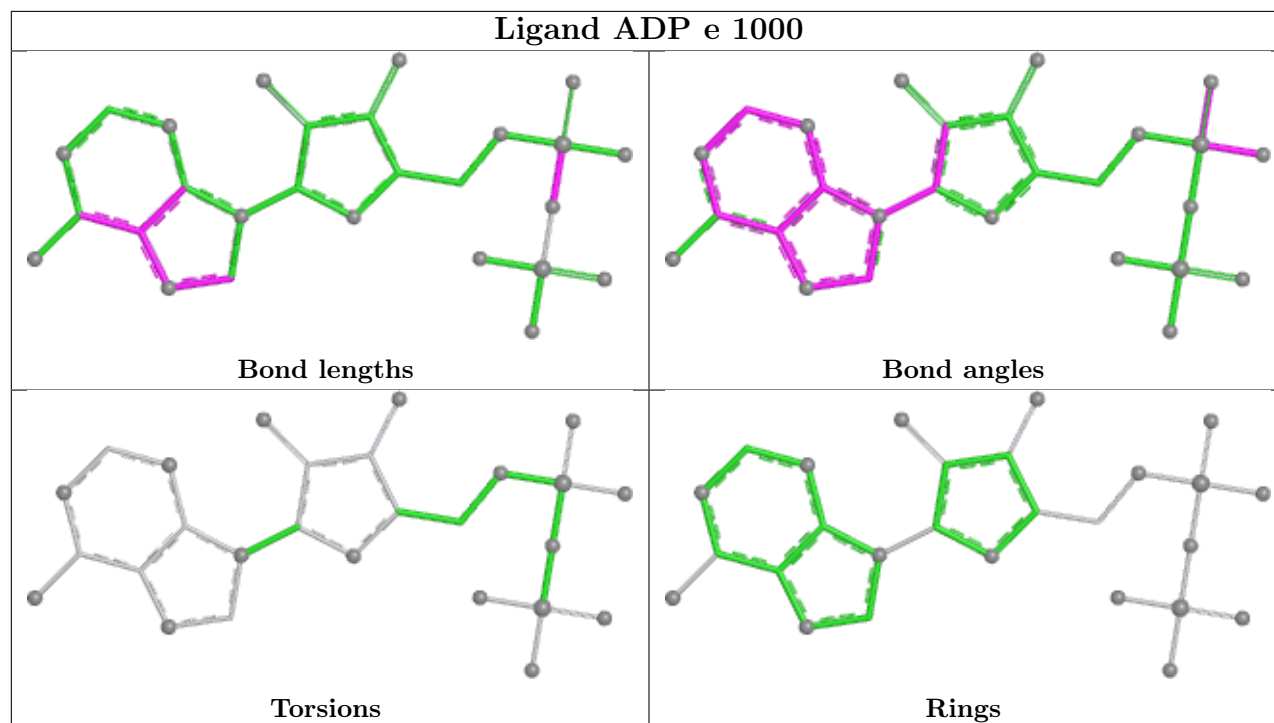
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5   | a     | 1002 | BEF  | 3       | 0            |
| 5   | c     | 1002 | BEF  | 3       | 0            |
| 5   | d     | 1002 | BEF  | 3       | 0            |

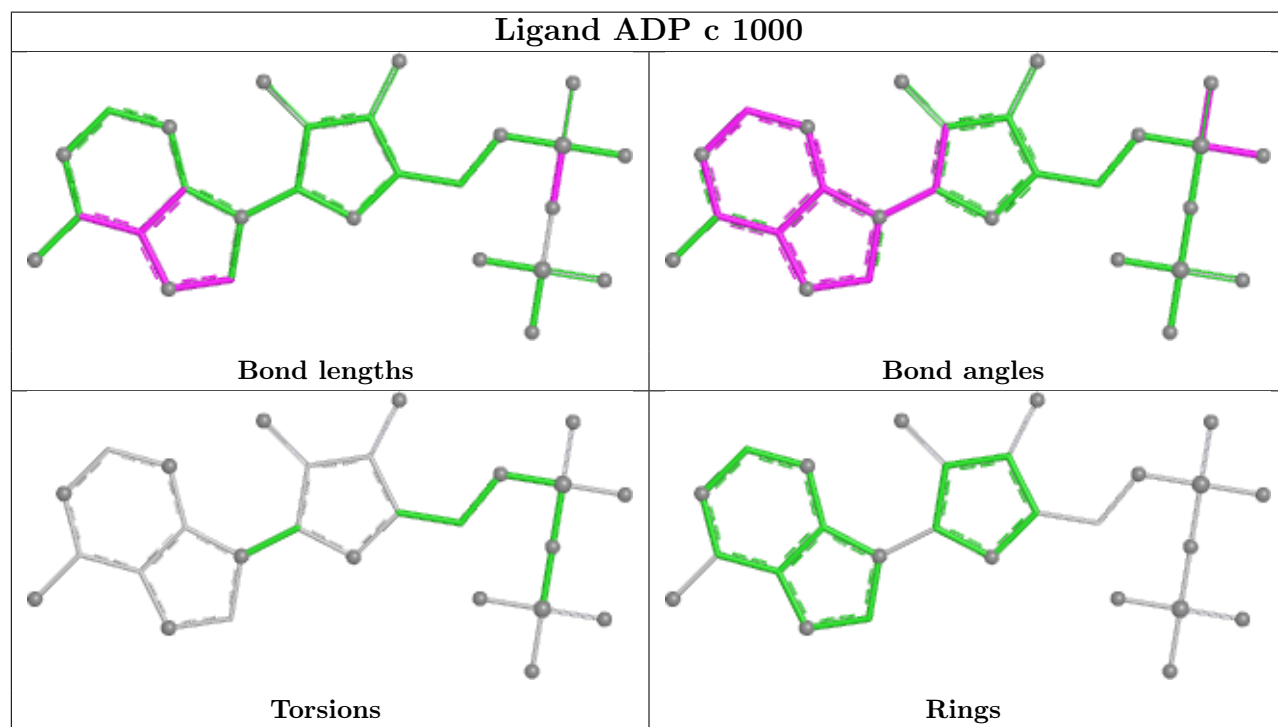
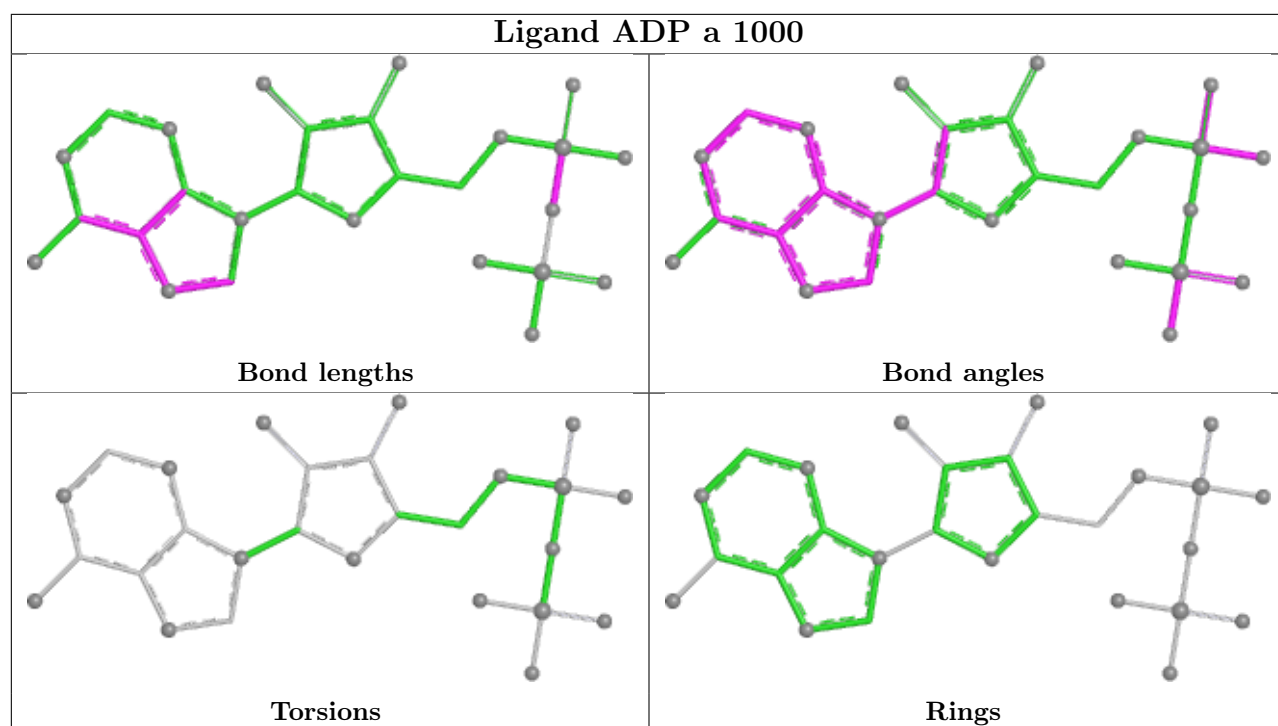
*Continued on next page...*

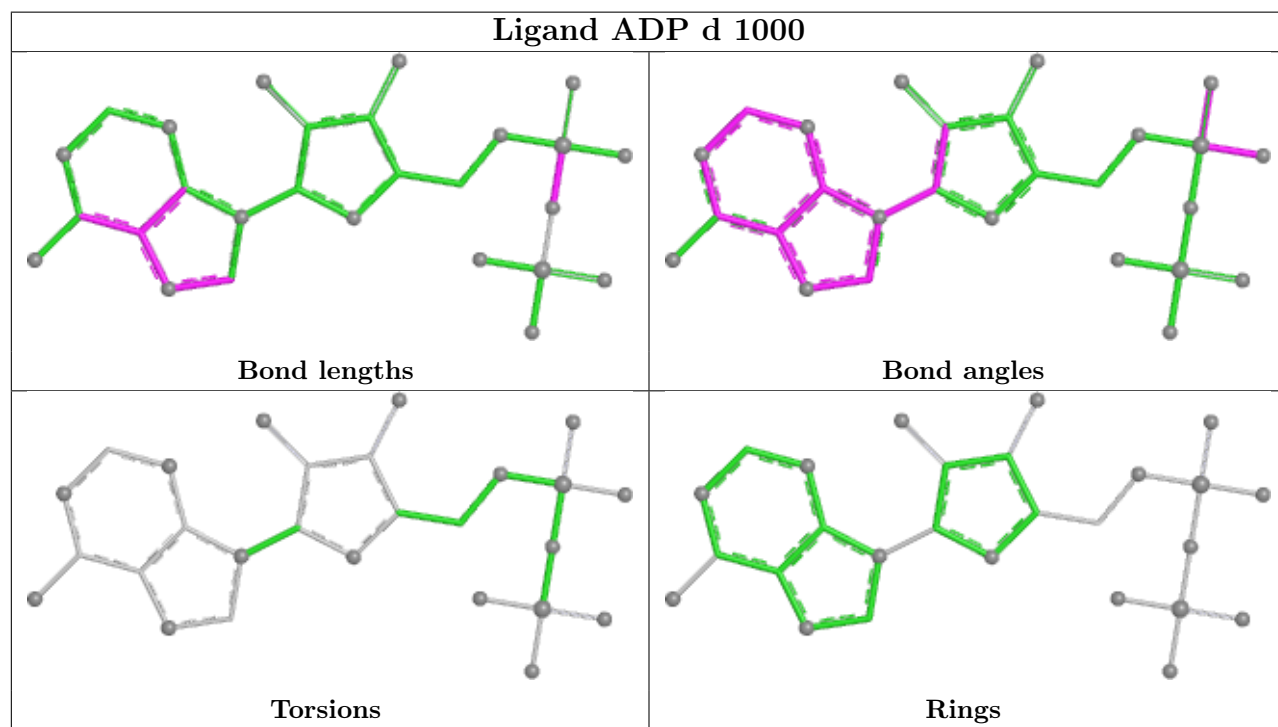
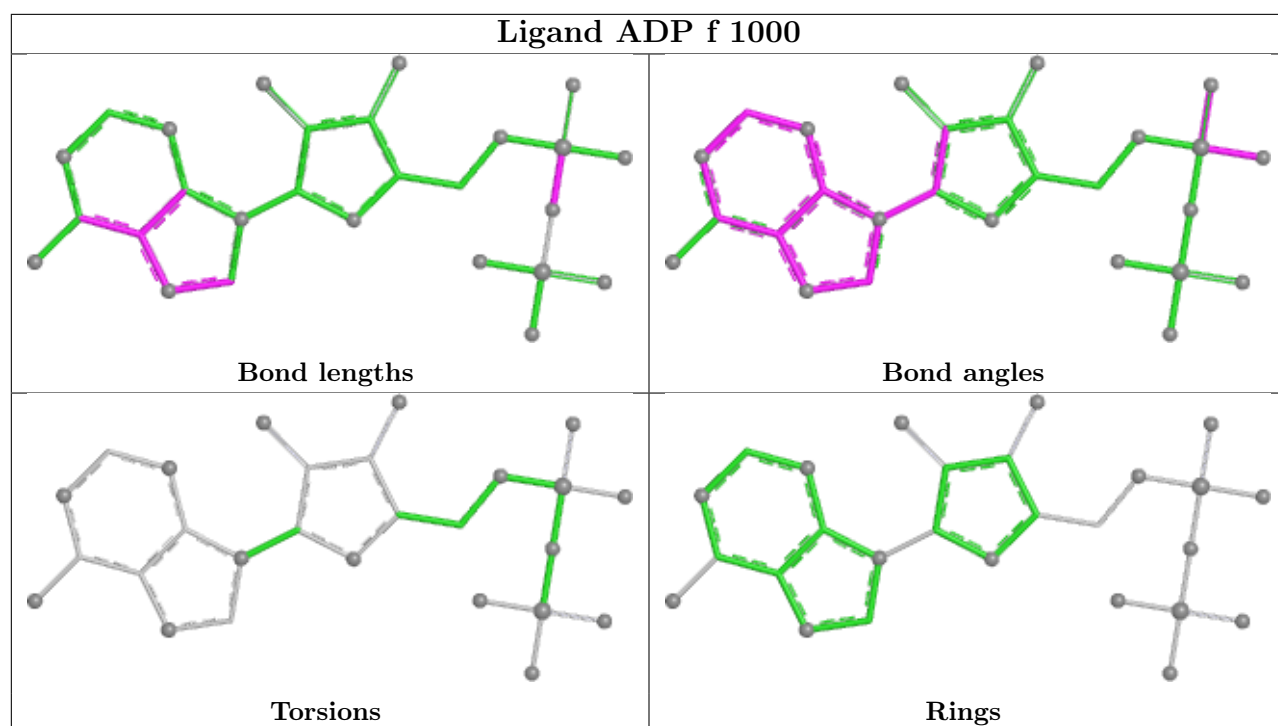
*Continued from previous page...*

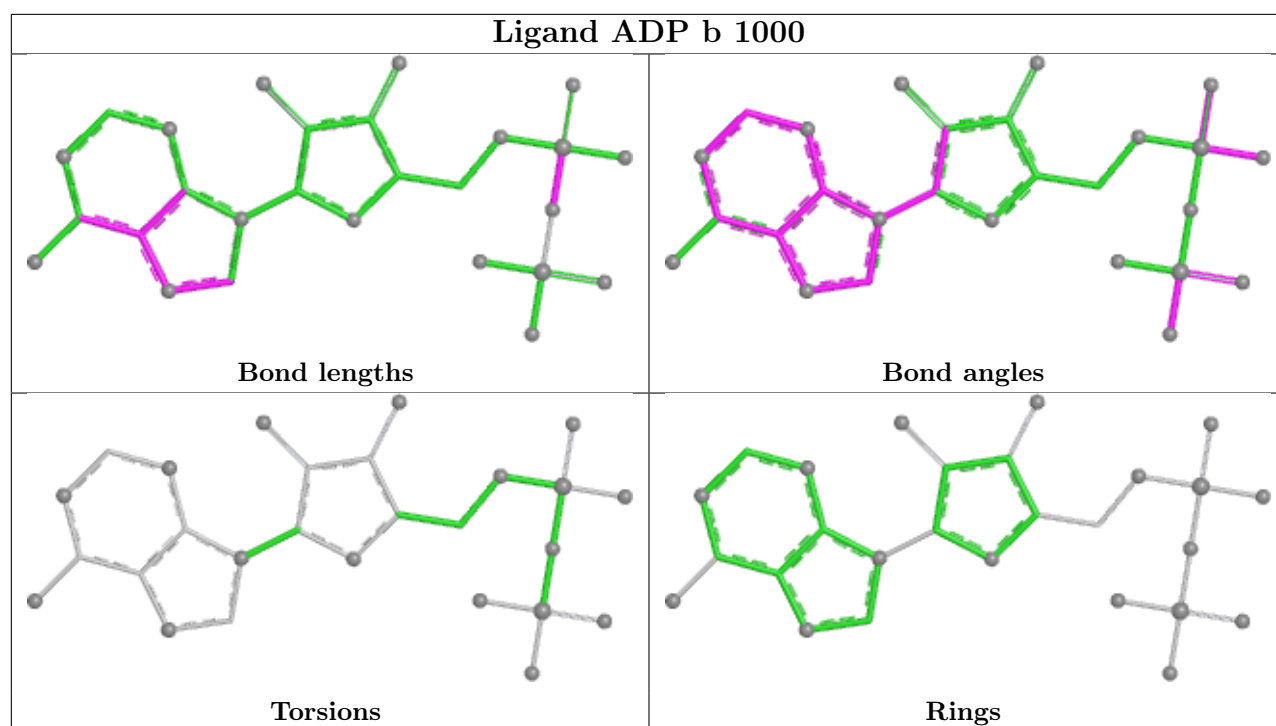
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | e     | 1000 | ADP  | 56      | 0            |
| 5   | e     | 1002 | BEF  | 3       | 0            |
| 5   | f     | 1002 | BEF  | 3       | 0            |
| 3   | a     | 1000 | ADP  | 58      | 0            |
| 3   | c     | 1000 | ADP  | 53      | 0            |
| 3   | f     | 1000 | ADP  | 62      | 0            |
| 3   | d     | 1000 | ADP  | 56      | 0            |
| 3   | b     | 1000 | ADP  | 59      | 0            |
| 5   | b     | 1002 | BEF  | 3       | 0            |

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

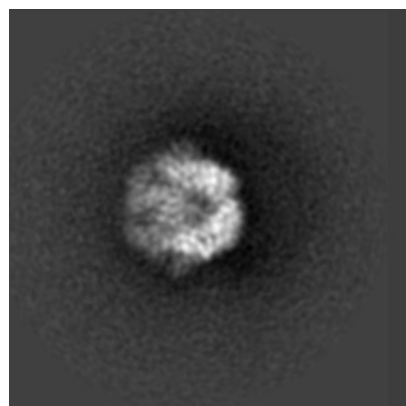
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27932. These allow visual inspection of the internal detail of the map and identification of artifacts.

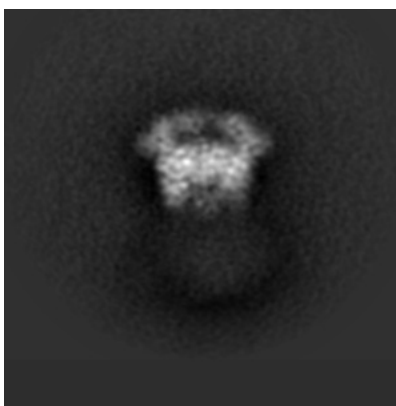
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

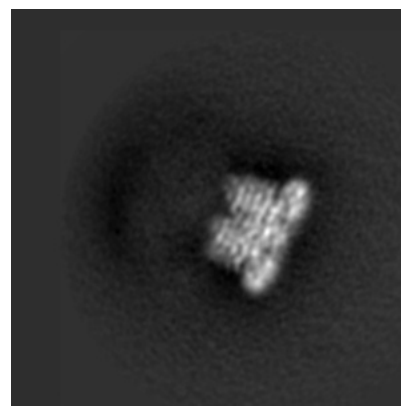
#### 6.1.1 Primary map



X

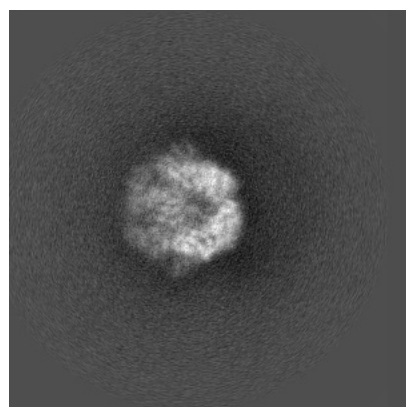


Y

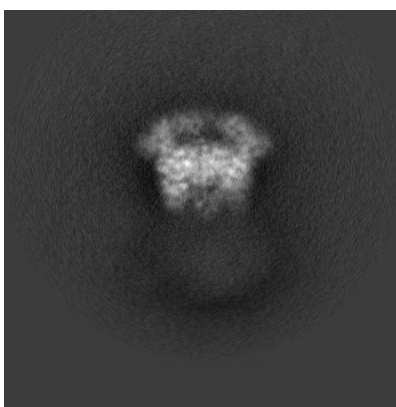


Z

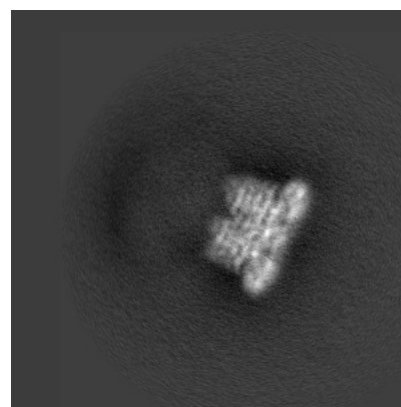
#### 6.1.2 Raw map



X



Y

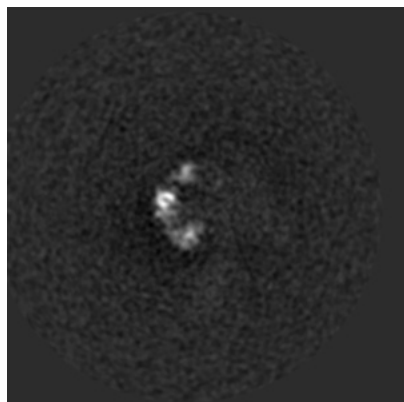


Z

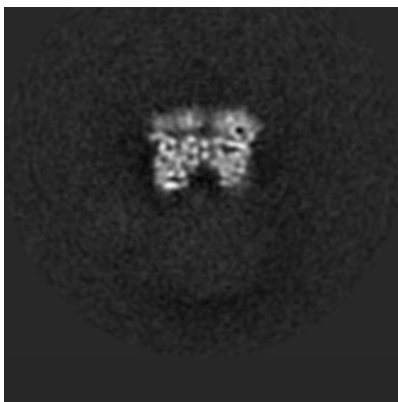
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

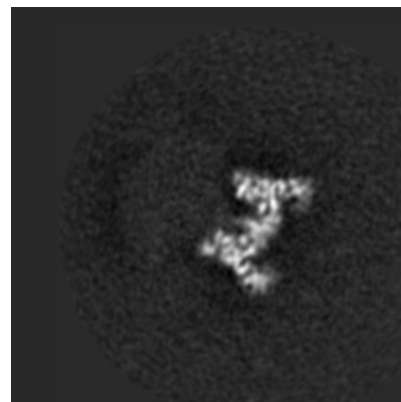
### 6.2.1 Primary map



X Index: 192

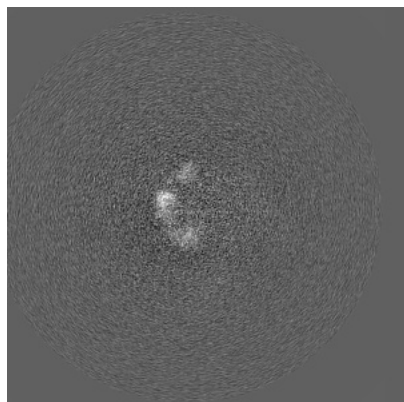


Y Index: 192

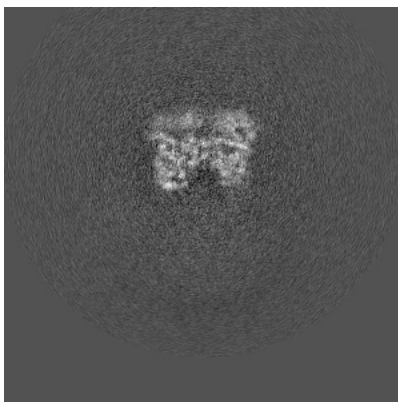


Z Index: 192

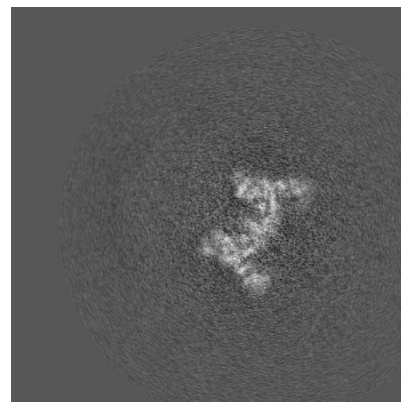
### 6.2.2 Raw map



X Index: 192



Y Index: 192

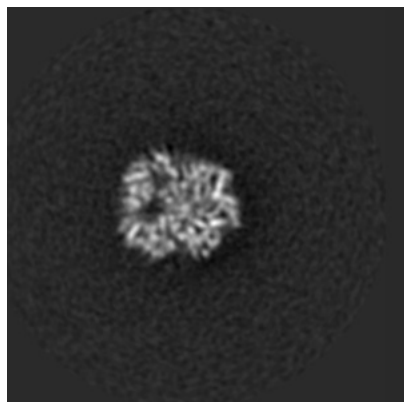


Z Index: 192

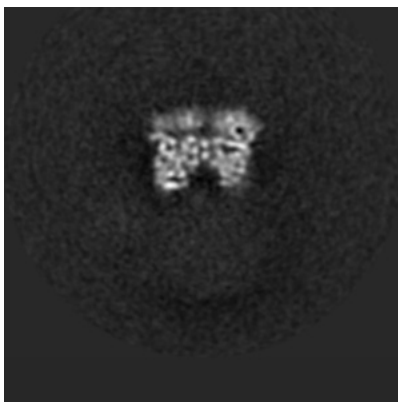
The images above show central slices of the map in three orthogonal directions.

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

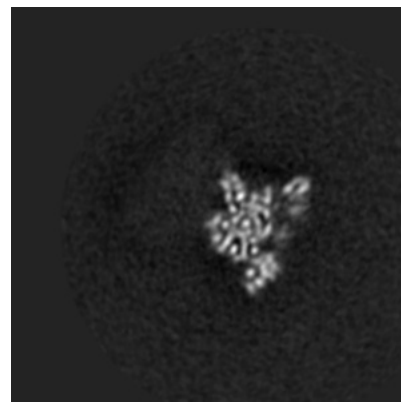
### 6.3.1 Primary map



X Index: 237

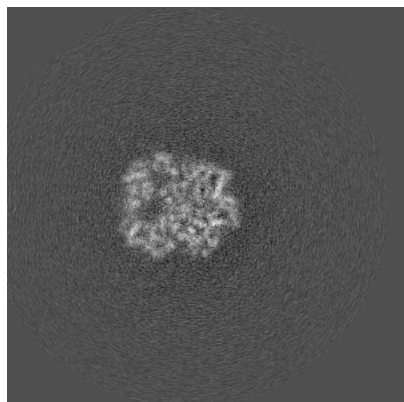


Y Index: 192

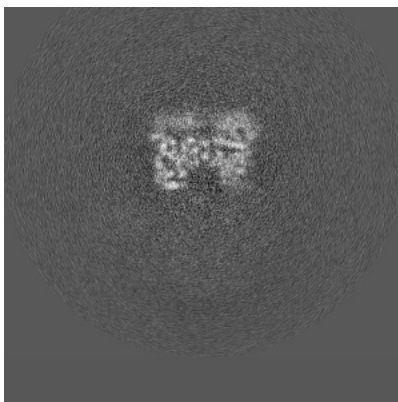


Z Index: 166

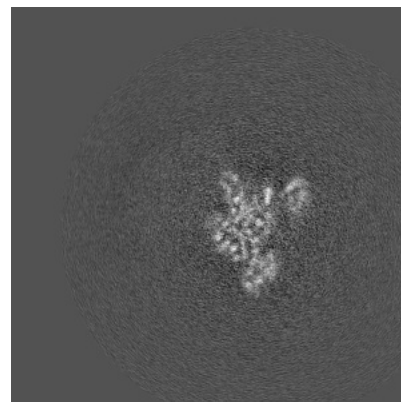
### 6.3.2 Raw map



X Index: 237



Y Index: 191

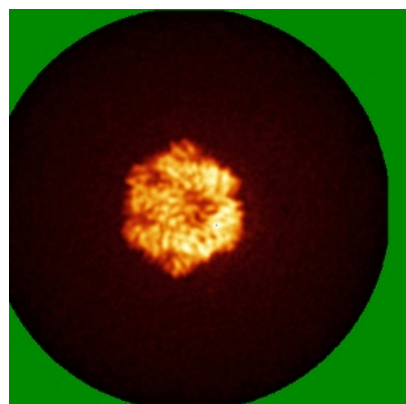


Z Index: 169

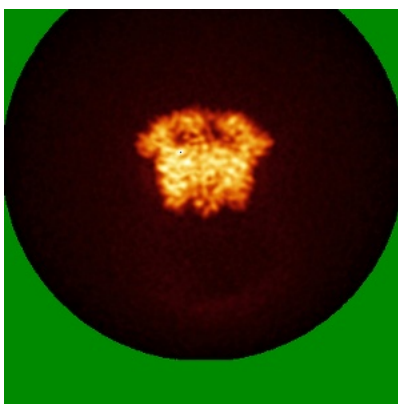
The images above show the largest variance slices of the map in three orthogonal directions.

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

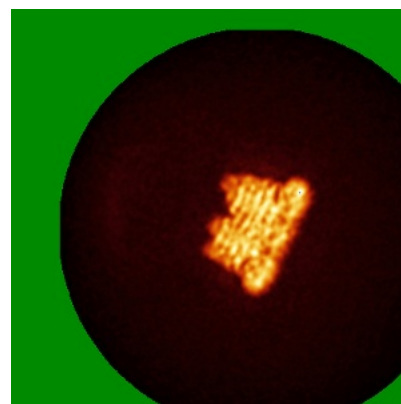
### 6.4.1 Primary map



X

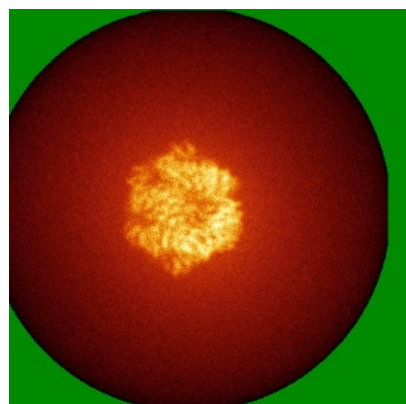


Y

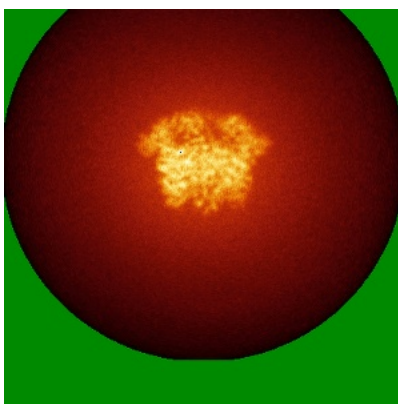


Z

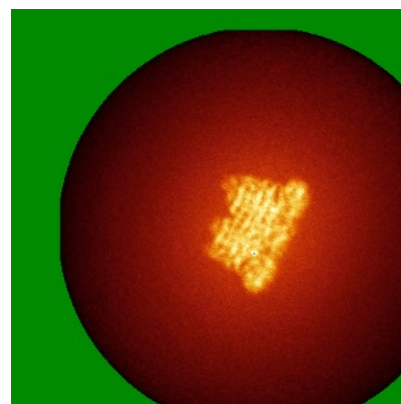
### 6.4.2 Raw map



X



Y

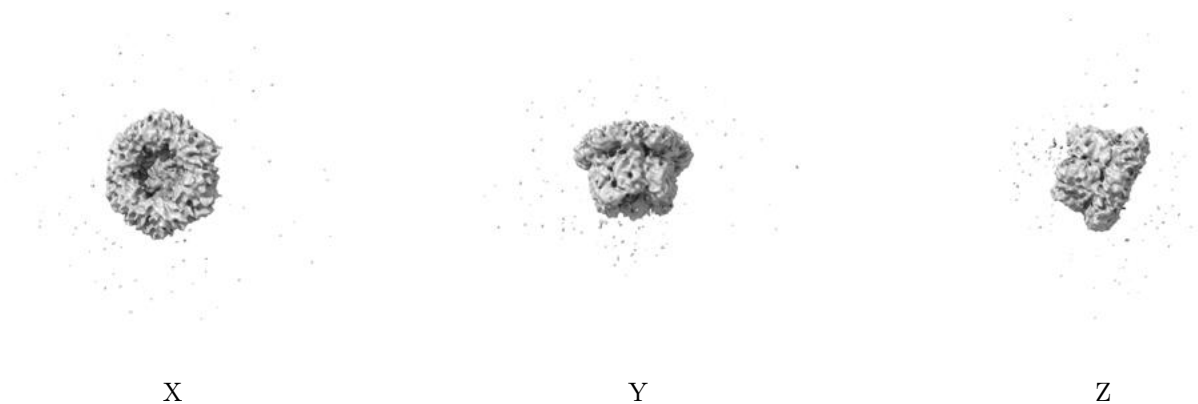


Z

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.

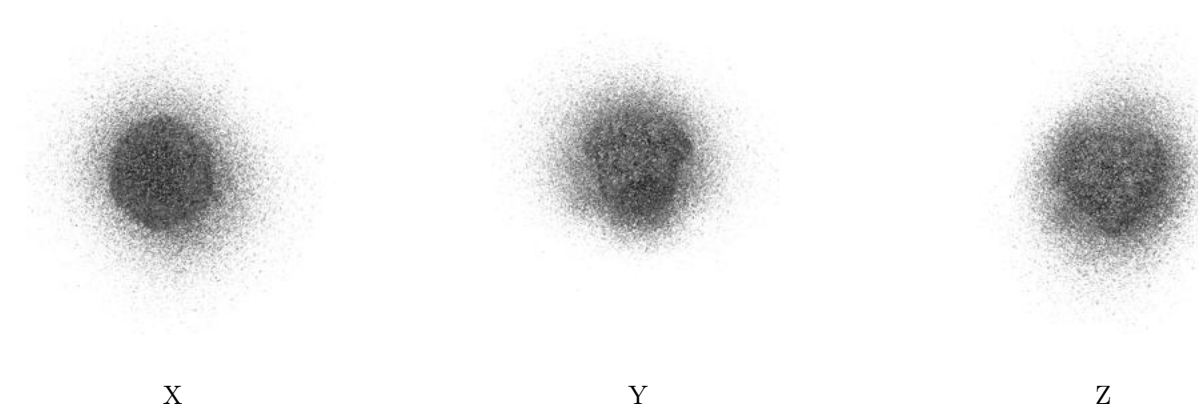
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

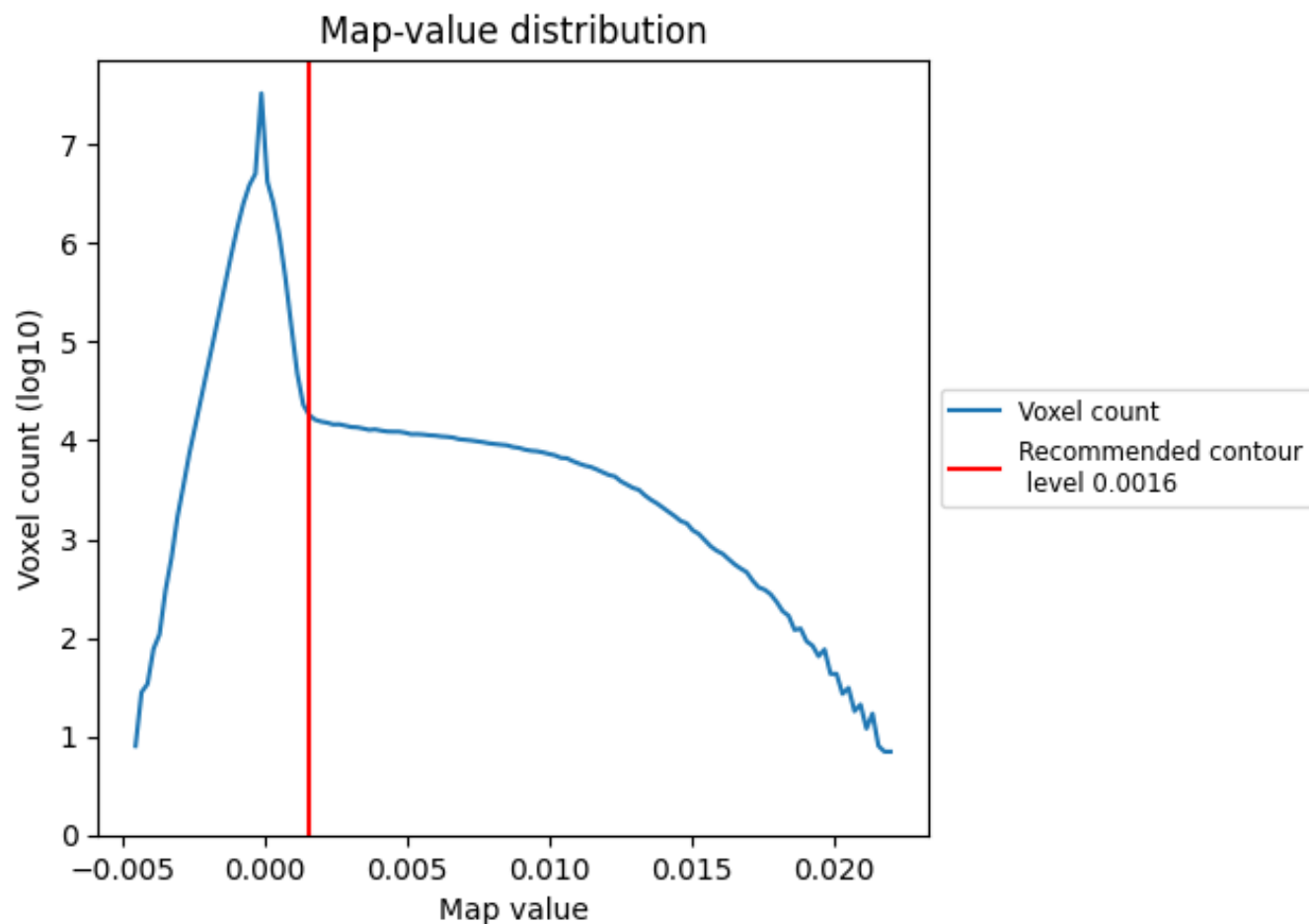
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

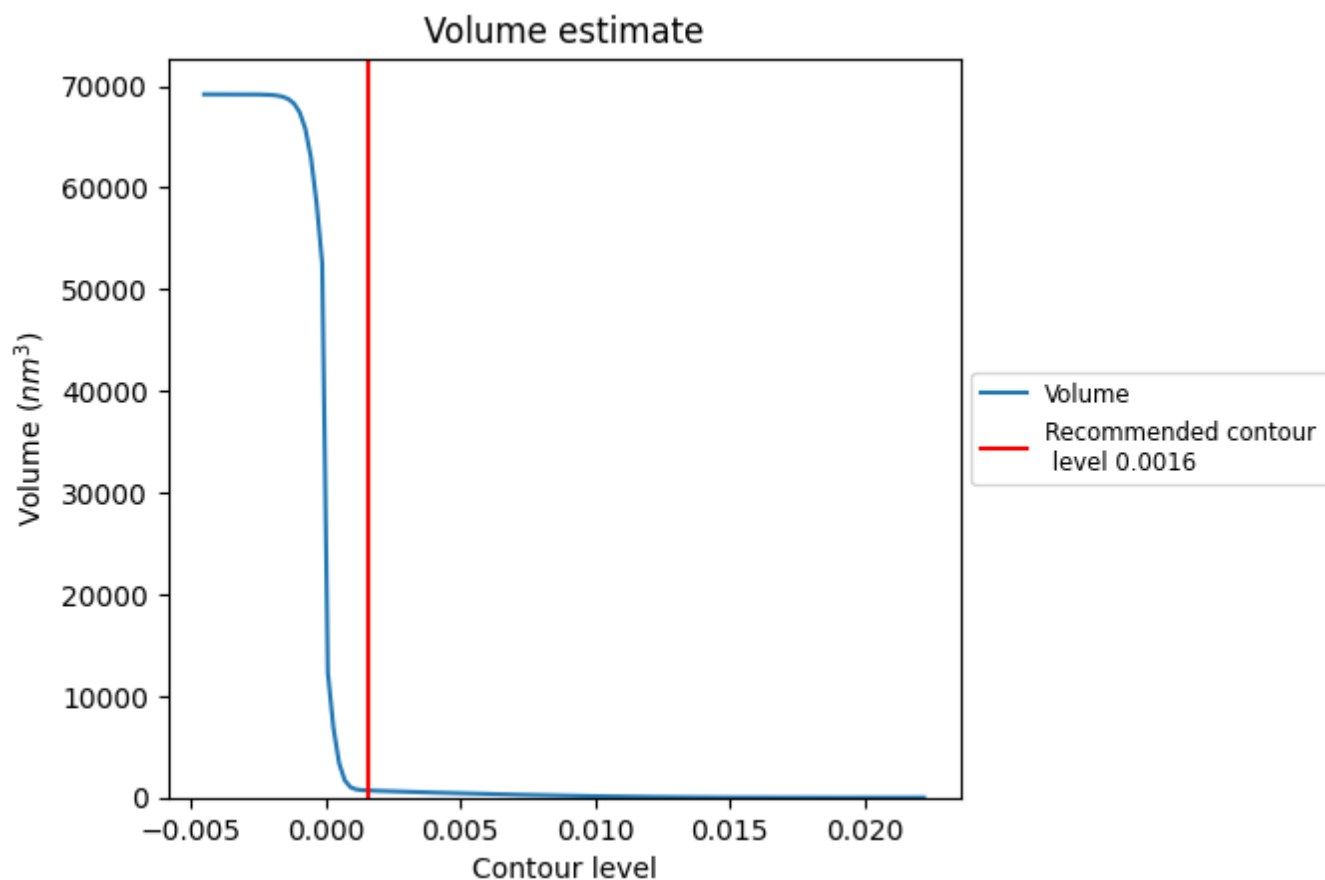
This section contains the results of statistical analysis of the map.

### 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.

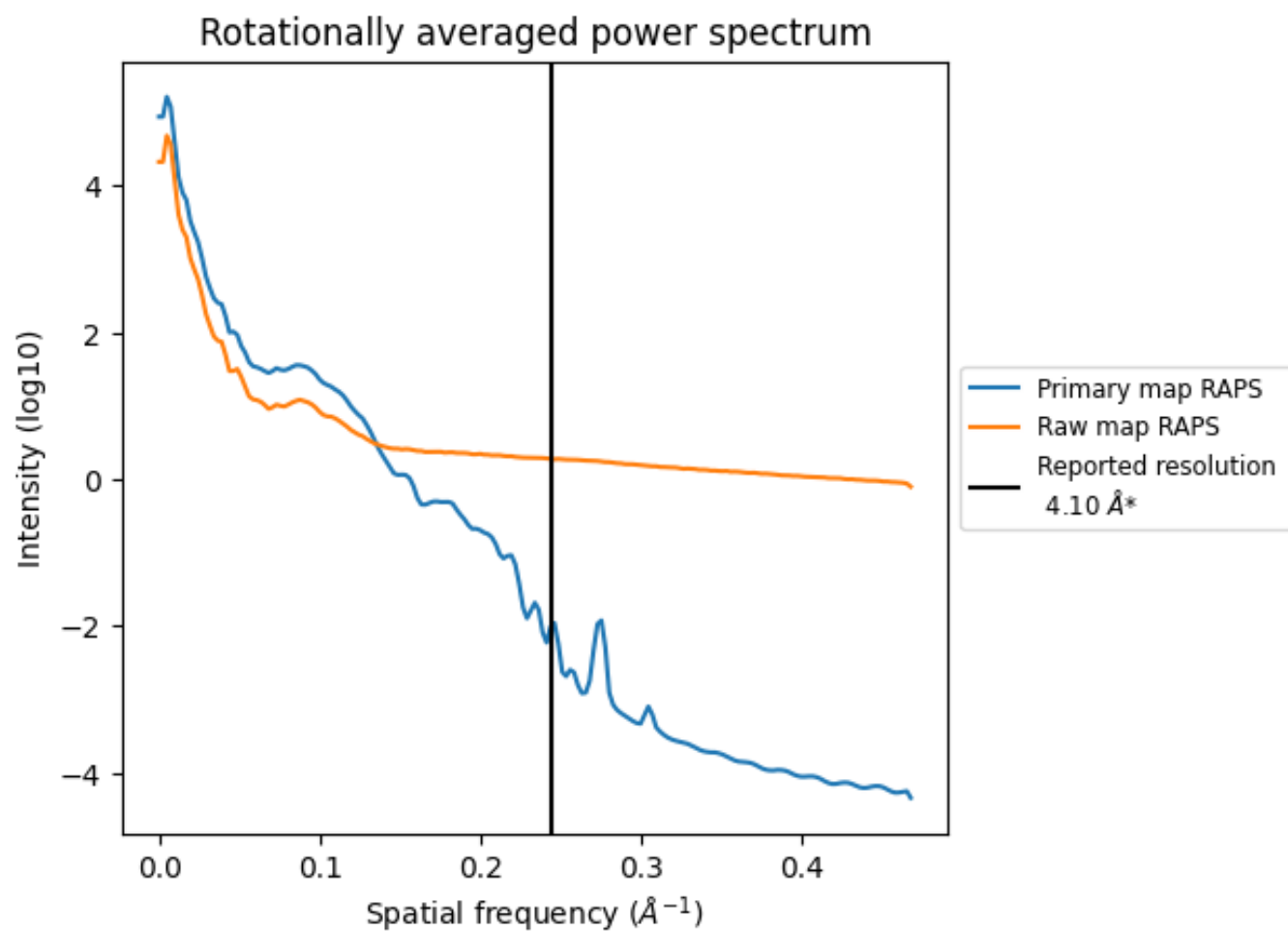
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 695 nm<sup>3</sup>; this corresponds to an approximate mass of 627 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 ⓘ

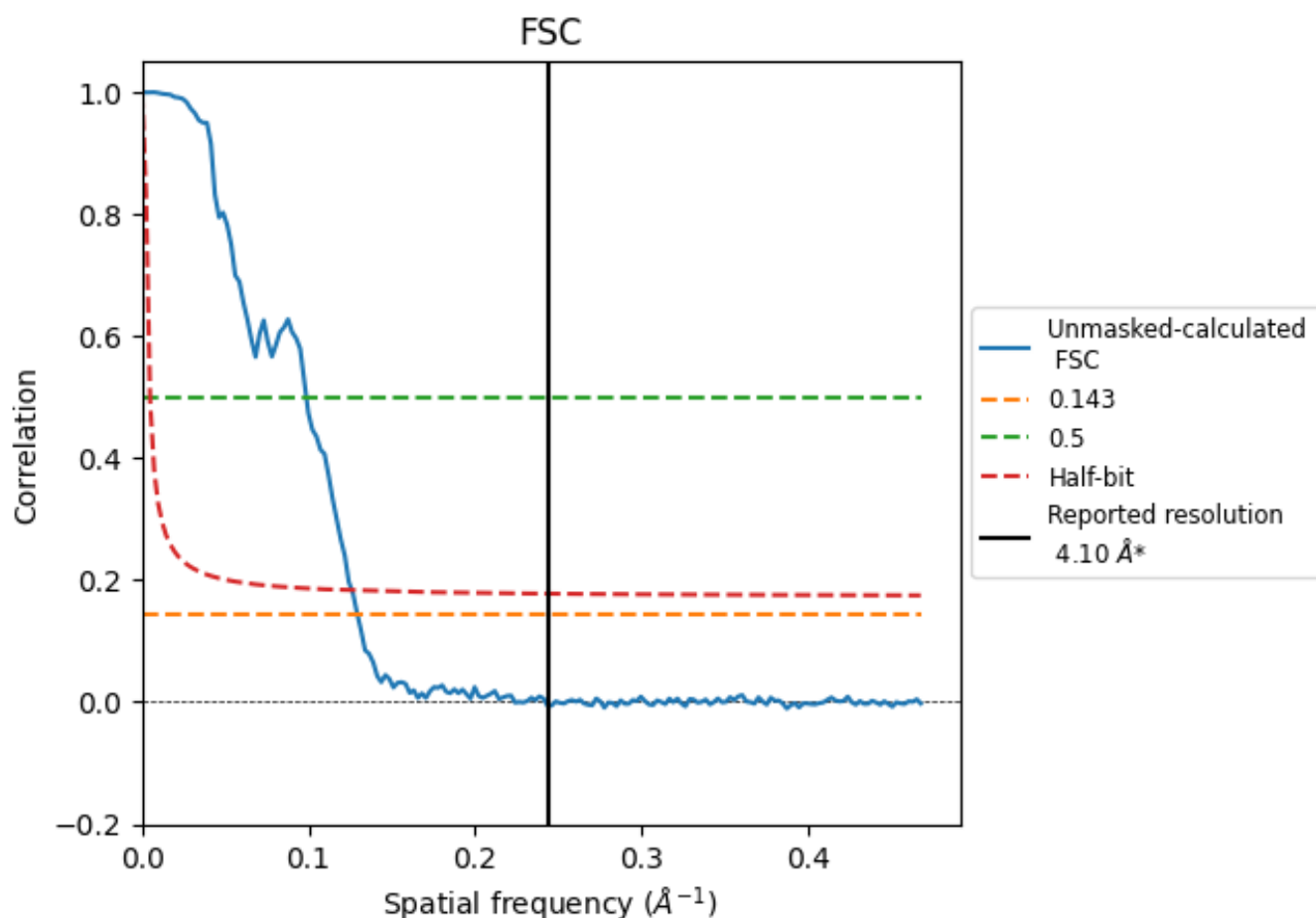


\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

## 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  $0.244 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

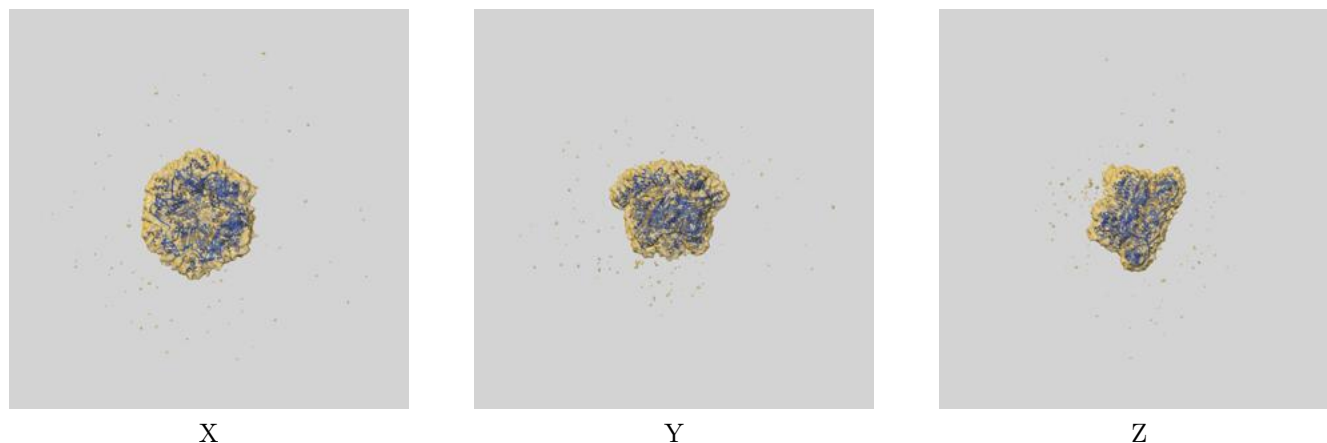
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 4.10                               | -     | -        |
| Author-provided FSC curve | -                                  | -     | -        |
| Unmasked-calculated*      | 7.73                               | 10.13 | 7.94     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.73 differs from the reported value 4.1 by more than 10 %

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

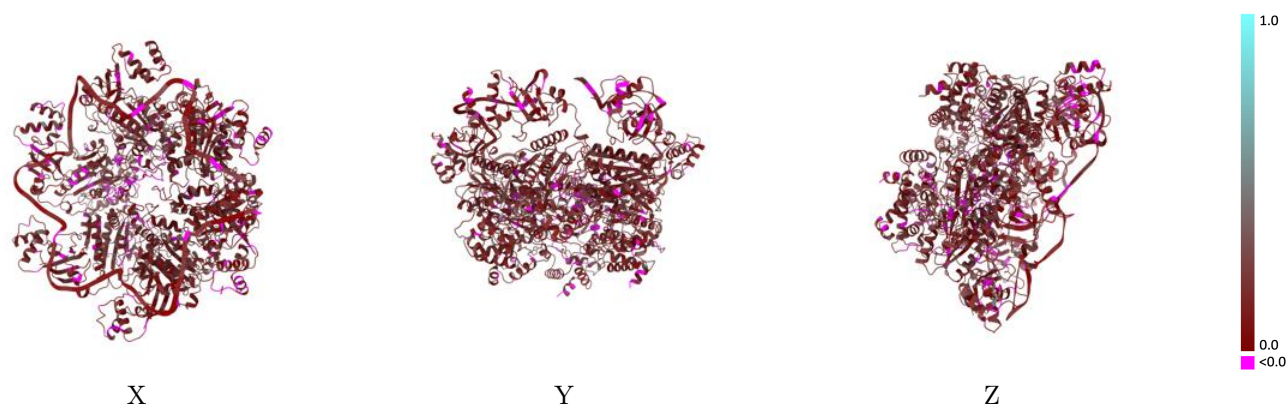
This section contains information regarding the fit between EMDB map EMD-27932 and PDB model 8E70. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



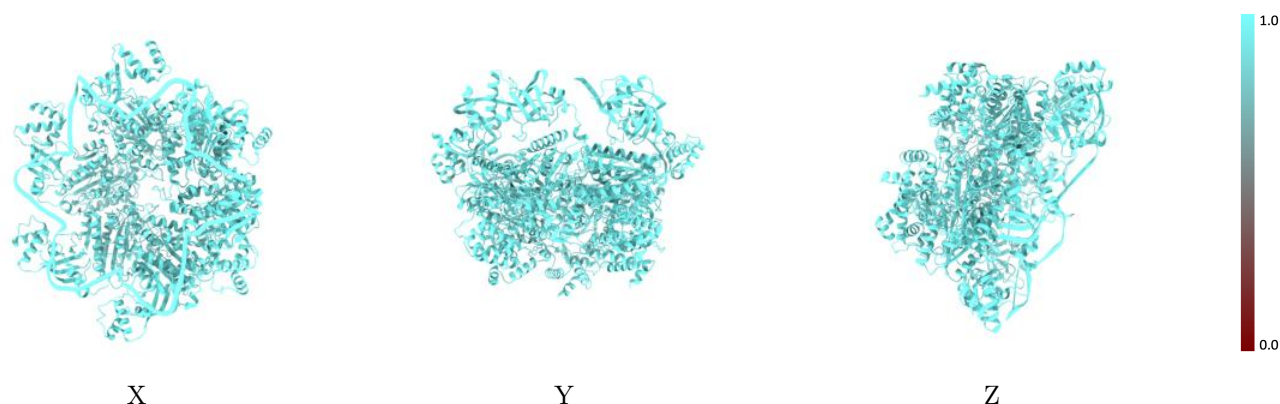
The images above show the 3D surface view of the map at the recommended contour level 0.0016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



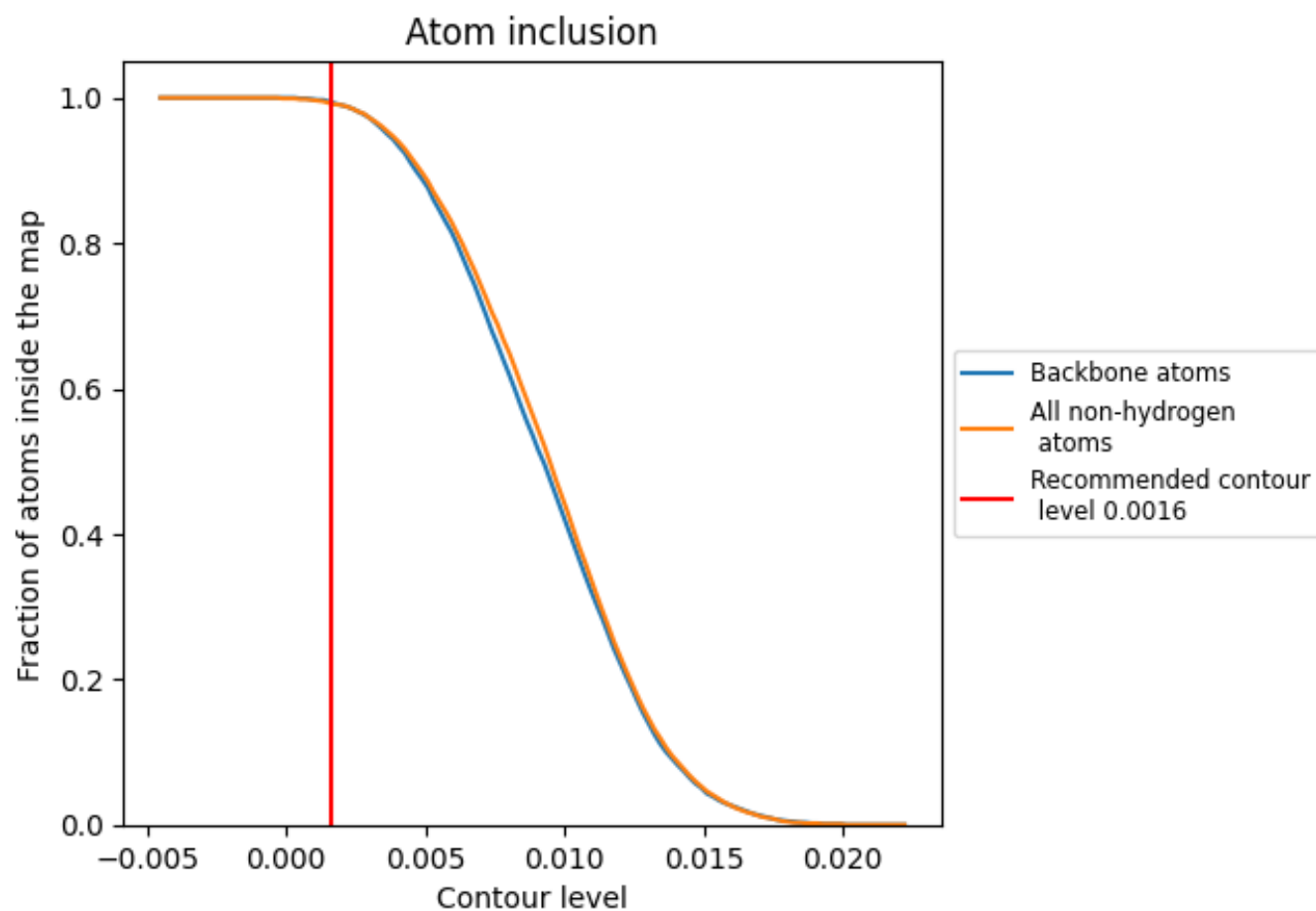
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0016).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.0016) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion               | Q-score                      |
|-------|------------------------------|------------------------------|
| All   | <div><div></div>0.9920</div> | <div><div></div>0.1530</div> |
| 8     | <div><div></div>0.9990</div> | <div><div></div>0.1180</div> |
| a     | <div><div></div>0.9900</div> | <div><div></div>0.1690</div> |
| b     | <div><div></div>0.9920</div> | <div><div></div>0.1600</div> |
| c     | <div><div></div>0.9950</div> | <div><div></div>0.1450</div> |
| d     | <div><div></div>0.9920</div> | <div><div></div>0.1460</div> |
| e     | <div><div></div>0.9950</div> | <div><div></div>0.1540</div> |
| f     | <div><div></div>0.9890</div> | <div><div></div>0.1550</div> |

1.0

0.0

<0.0