



## Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 02:29 PM JST

PDB ID : 7X3T / pdb\_00007x3t  
EMDB ID : EMD-32992  
Title : Cryo-EM structure of ISW1a-dinucleosome  
Authors : Lifei, L.; Kangjing, C.; Chen, Z.  
Deposited on : 2022-03-01  
Resolution : 5.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

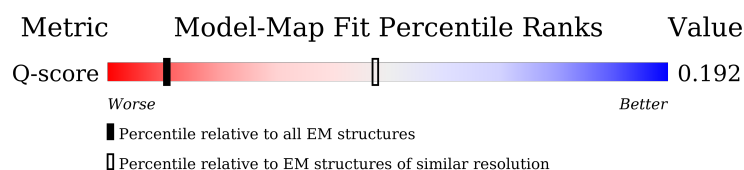
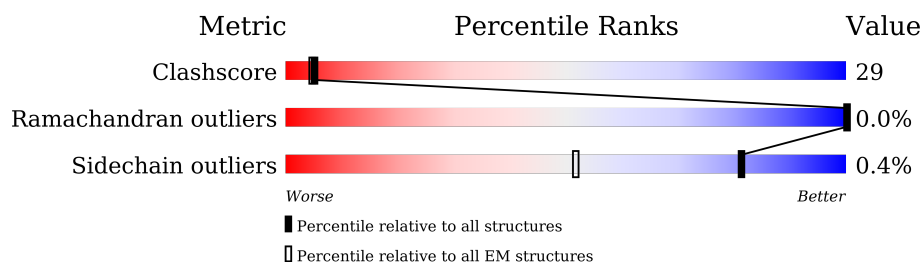
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.40 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 538 ( 4.90 - 5.90 )                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 136    |                  |
| 1   | E     | 136    |                  |
| 1   | K     | 136    |                  |
| 1   | O     | 136    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | B     | 103    |                  |
| 2   | F     | 103    |                  |
| 2   | L     | 103    |                  |
| 2   | P     | 103    |                  |
| 3   | C     | 130    |                  |
| 3   | G     | 130    |                  |
| 3   | M     | 130    |                  |
| 3   | Q     | 130    |                  |
| 4   | D     | 126    |                  |
| 4   | H     | 126    |                  |
| 4   | N     | 126    |                  |
| 4   | R     | 126    |                  |
| 5   | I     | 354    |                  |
| 6   | J     | 354    |                  |
| 7   | U     | 624    |                  |
| 8   | V     | 1062   |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 10  | BEF  | V     | 1202 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 37283 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | A     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 801   | 506 | 153 | 139 | 3 |         |       |
| 1   | E     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 779   | 492 | 148 | 136 | 3 |         |       |
| 1   | K     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 801   | 506 | 153 | 139 | 3 |         |       |
| 1   | O     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 779   | 492 | 148 | 136 | 3 |         |       |

- Molecule 2 is a protein called Histone H4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | B     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 653   | 413 | 127 | 112 | 1 |         |       |
| 2   | F     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 672   | 424 | 130 | 117 | 1 |         |       |
| 2   | L     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 707   | 445 | 143 | 118 | 1 |         |       |
| 2   | P     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 632   | 398 | 122 | 111 | 1 |         |       |

- Molecule 3 is a protein called Histone H2A.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 3   | C     | 107      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 811   | 510 | 158 | 143 |         |       |
| 3   | G     | 107      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 815   | 513 | 159 | 143 |         |       |
| 3   | M     | 107      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 811   | 510 | 158 | 143 |         |       |
| 3   | Q     | 107      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 815   | 513 | 159 | 143 |         |       |

- Molecule 4 is a protein called Histone H2B 1.1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 717   | 450 | 128 | 137 | 2 |         |       |
| 4   | H     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 725   | 456 | 130 | 137 | 2 |         |       |
| 4   | N     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 717   | 450 | 128 | 137 | 2 |         |       |
| 4   | R     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 725   | 456 | 130 | 137 | 2 |         |       |

- Molecule 5 is a DNA chain called DNA (343-MER).

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 5   | I     | 339      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 6918  | 3286 | 1256 | 2037 | 339 |         |       |

- Molecule 6 is a DNA chain called DNA(343-MER).

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 6   | J     | 339      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 6981  | 3306 | 1305 | 2031 | 339 |         |       |

- Molecule 7 is a protein called ISWI one complex protein 3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | U     | 590      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4840  | 3114 | 816 | 895 | 15 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| U     | 126     | MET      | -      | initiating methionine | UNP P43596 |

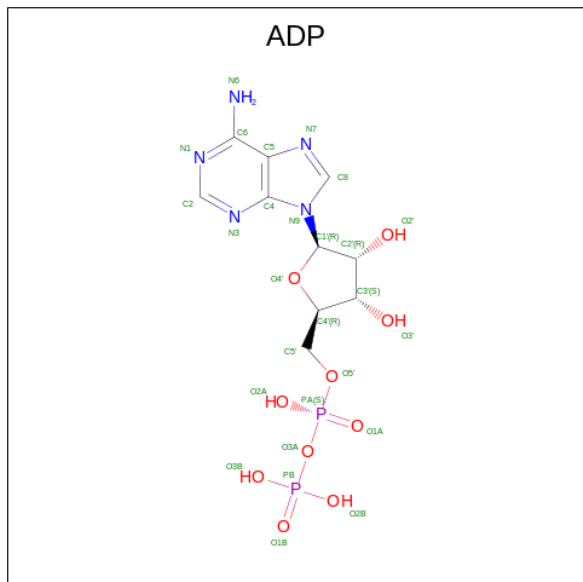
- Molecule 8 is a protein called ISWI chromatin-remodeling complex ATPase ISW1.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 8   | V     | 792      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6552  | 4175 | 1132 | 1223 | 22 |         |       |

There is a discrepancy between the modelled and reference sequences:

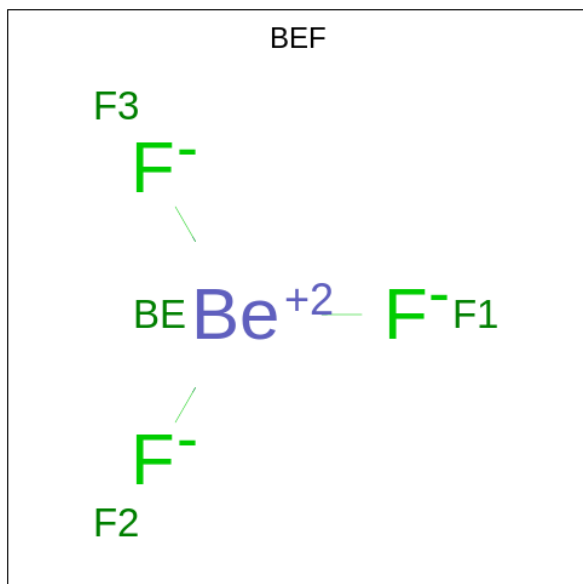
| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| V     | 68      | MET      | -      | initiating methionine | UNP P38144 |

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 9   | V     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula:  $BeF_3$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 10  | V     | 1        | Total | Be | F | 0       |
|     |       |          | 4     | 1  | 3 |         |

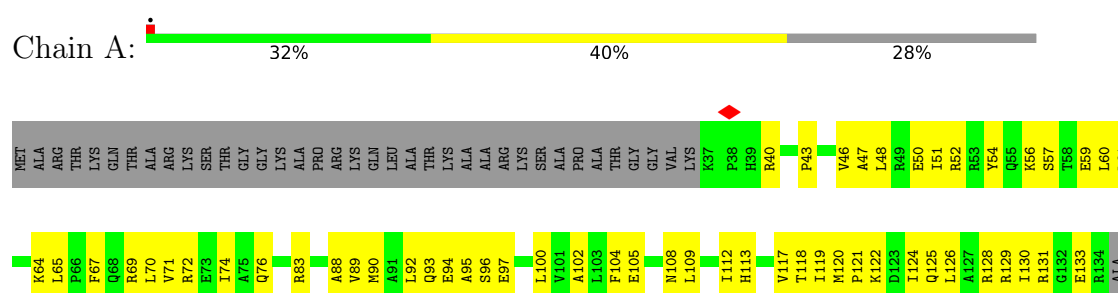
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

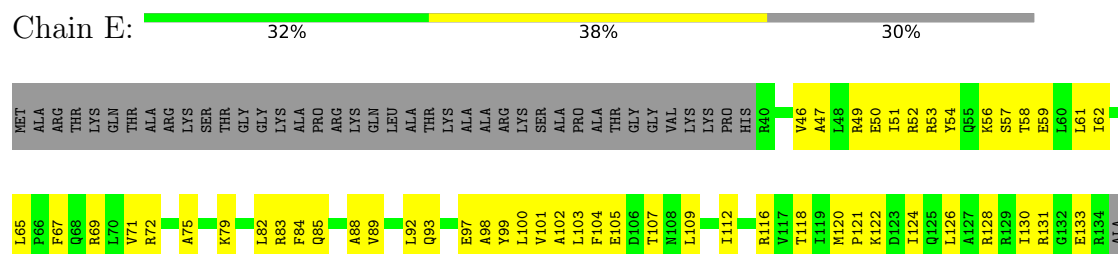
### 3 Residue-property plots

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

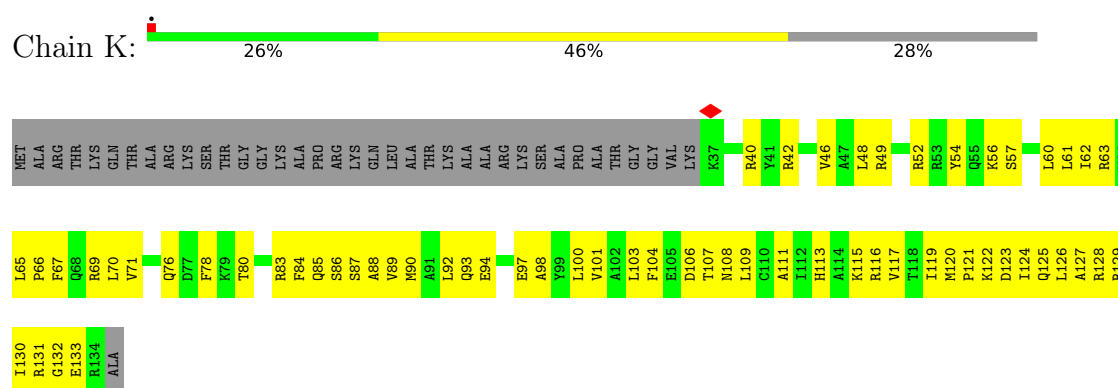
#### • Molecule 1: Histone H3



#### • Molecule 1: Histone H3



#### • Molecule 1: Histone H3



#### • Molecule 1: Histone H3



- Molecule 2: Histone H4



- Molecule 2: Histone H4



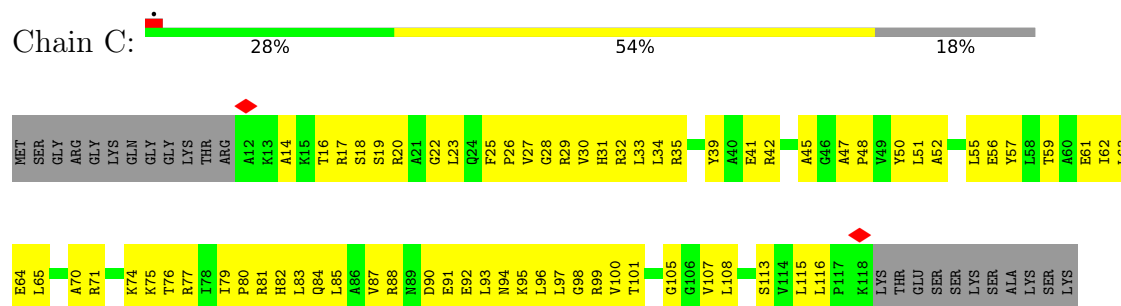
- Molecule 2: Histone H4



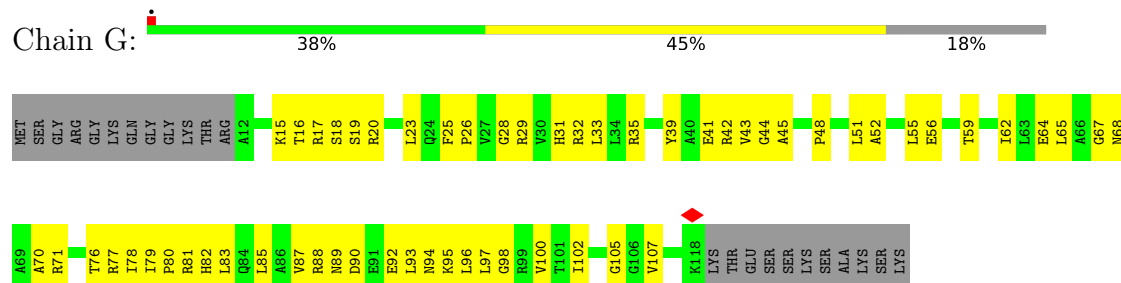
- Molecule 2: Histone H4



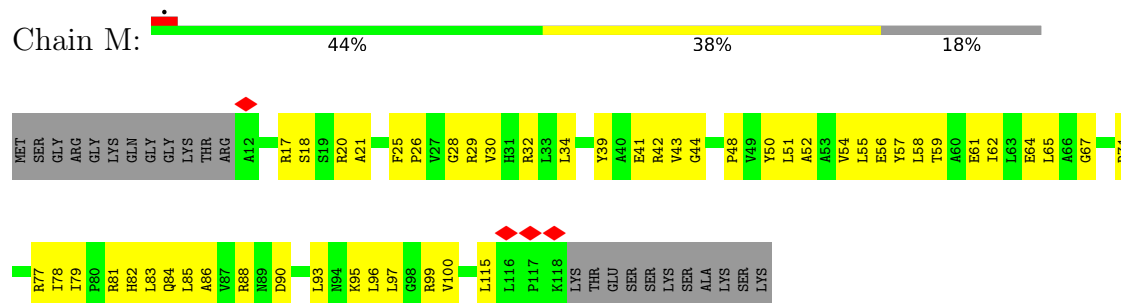
- Molecule 3: Histone H2A



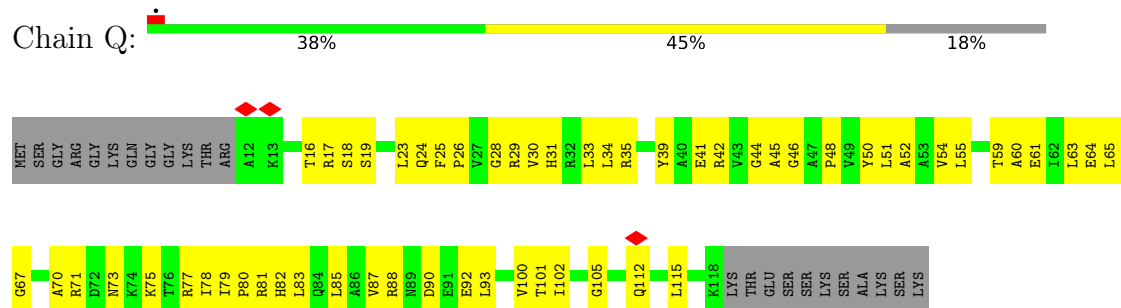
- Molecule 3: Histone H2A



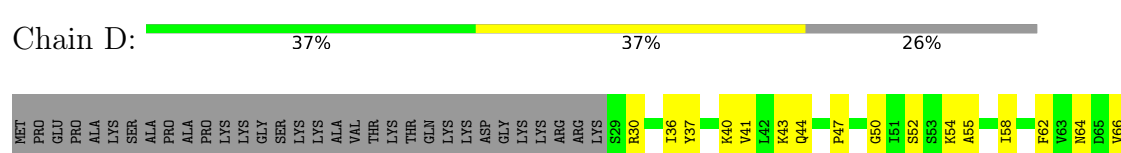
- Molecule 3: Histone H2A

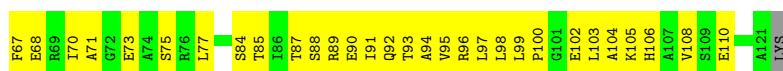


- Molecule 3: Histone H2A



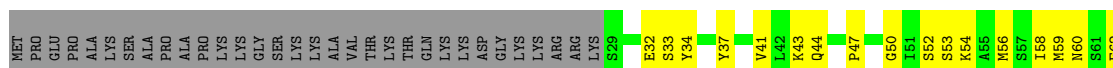
- Molecule 4: Histone H2B 1.1





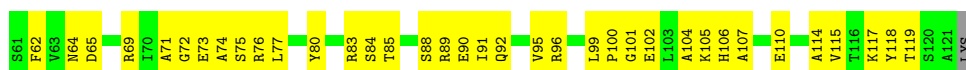
• Molecule 4: Histone H2B 1.1

Chain H: 40% 34% 26%



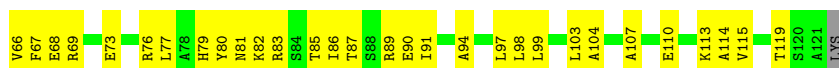
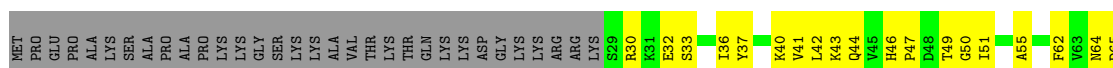
• Molecule 4: Histone H2B 1.1

Chain N: 29% 44% 26%



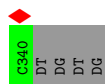
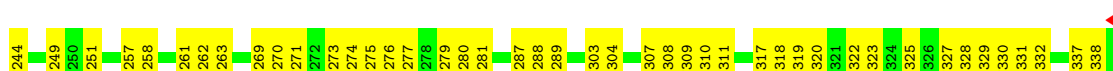
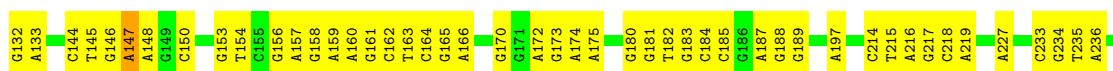
• Molecule 4: Histone H2B 1.1

Chain R: 35% 39% 26%

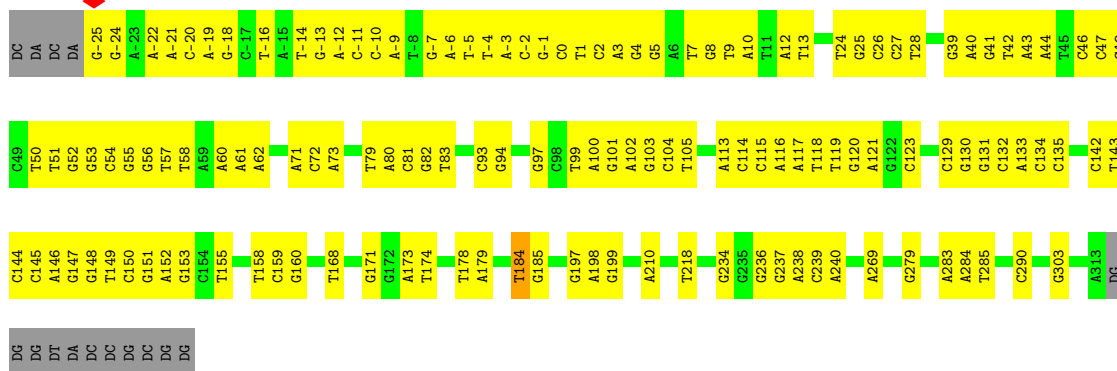


• Molecule 5: DNA (343-MER)

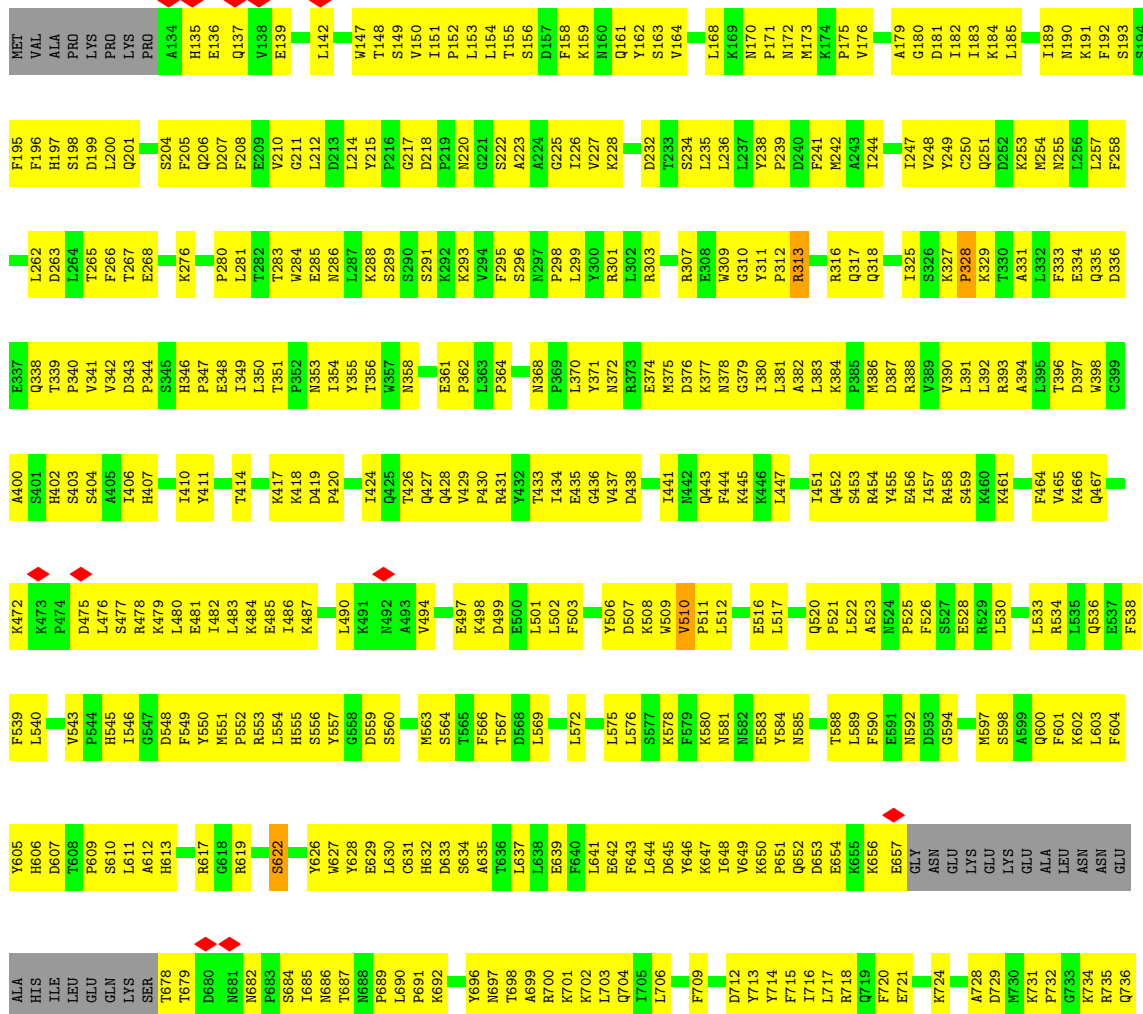
Chain I: 61% 34%



Chain J:  57% 38% .

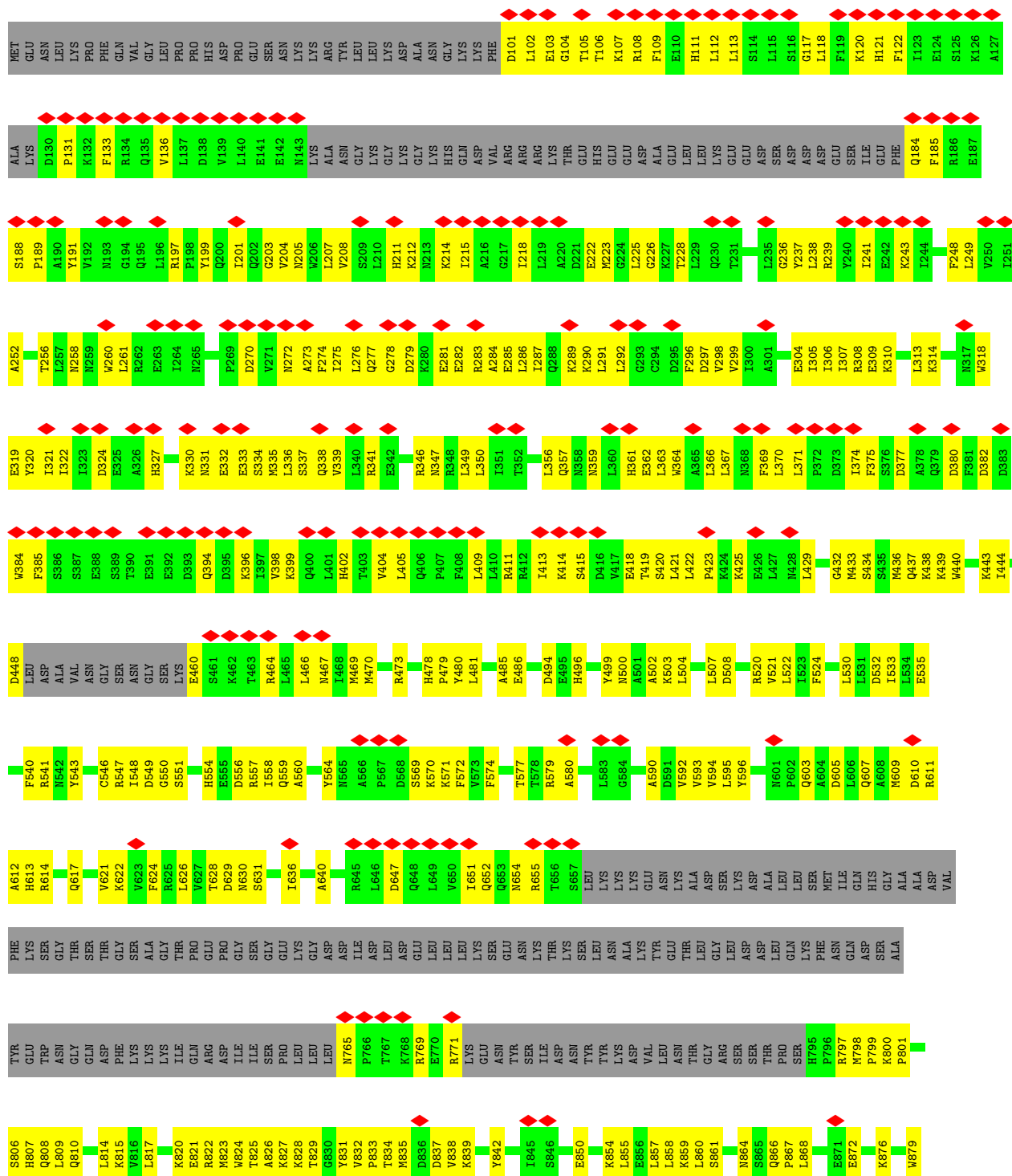


Chain U:  33% 61% 5%





• Molecule 8: ISWI chromatin-remodeling complex ATPase ISW1





## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, Not provided             |           |
| Number of particles used             | 66852                           | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | NONE                            | Depositor |
| Microscope                           | FEI TITAN KRIOS                 | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                              | Depositor |
| Minimum defocus (nm)                 | 1400                            | Depositor |
| Maximum defocus (nm)                 | 1800                            | Depositor |
| Magnification                        | Not provided                    |           |
| Image detector                       | GATAN K3 (6k x 4k)              | Depositor |
| Maximum map value                    | 0.030                           | Depositor |
| Minimum map value                    | -0.010                          | Depositor |
| Average map value                    | 0.000                           | Depositor |
| Map value standard deviation         | 0.001                           | Depositor |
| Recommended contour level            | 0.0048                          | Depositor |
| Map size ( $\text{\AA}$ )            | 389.69998, 389.69998, 389.69998 | wwPDB     |
| Map dimensions                       | 360, 360, 360                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.0825, 1.0825, 1.0825          | Depositor |

## 5 Model quality [i](#)

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

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

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.45         | 0/813          | 0.72        | 0/1093          |
| 1   | E     | 0.45         | 0/789          | 0.64        | 0/1059          |
| 1   | K     | 0.39         | 0/813          | 0.60        | 0/1093          |
| 1   | O     | 0.34         | 0/789          | 0.58        | 1/1059 (0.1%)   |
| 2   | B     | 0.62         | 0/660          | 0.85        | 0/885           |
| 2   | F     | 0.52         | 0/680          | 0.80        | 0/912           |
| 2   | L     | 0.42         | 0/715          | 0.68        | 0/955           |
| 2   | P     | 0.32         | 0/639          | 0.57        | 0/855           |
| 3   | C     | 0.46         | 0/821          | 0.66        | 0/1112          |
| 3   | G     | 0.44         | 0/825          | 0.63        | 0/1116          |
| 3   | M     | 0.34         | 0/821          | 0.58        | 0/1112          |
| 3   | Q     | 0.32         | 0/825          | 0.54        | 0/1116          |
| 4   | D     | 0.53         | 0/728          | 0.70        | 0/983           |
| 4   | H     | 0.48         | 0/736          | 0.67        | 0/991           |
| 4   | N     | 0.37         | 0/728          | 0.59        | 0/983           |
| 4   | R     | 0.35         | 0/736          | 0.54        | 0/991           |
| 5   | I     | 0.41         | 0/7753         | 0.64        | 8/11956 (0.1%)  |
| 6   | J     | 0.37         | 0/7839         | 0.60        | 2/12105 (0.0%)  |
| 7   | U     | 0.37         | 1/4962 (0.0%)  | 0.60        | 2/6709 (0.0%)   |
| 8   | V     | 0.24         | 0/6680         | 0.50        | 0/8996          |
| All | All   | 0.38         | 1/39352 (0.0%) | 0.61        | 13/56081 (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 |
|-----|-------|---------------------|---------------------|
| 8   | V     | 0                   | 1                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 7   | U     | 510 | VAL  | CA-CB | -8.24 | 1.49        | 1.54     |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | I     | 123 | DC   | C4'-C3'-O3' | 7.60  | 121.40      | 110.00   |
| 1   | O     | 117 | VAL  | N-CA-C      | -6.69 | 106.78      | 113.20   |
| 5   | I     | 180 | DG   | C2'-C3'-O3' | -6.39 | 101.91      | 111.50   |
| 6   | J     | 184 | DT   | C4'-C3'-O3' | 6.30  | 119.45      | 110.00   |
| 5   | I     | 148 | DA   | C2'-C3'-O3' | -6.22 | 102.17      | 111.50   |
| 5   | I     | 147 | DA   | C4'-C3'-O3' | 6.15  | 119.23      | 110.00   |
| 5   | I     | 99  | DG   | C2'-C3'-O3' | -6.04 | 102.44      | 111.50   |
| 7   | U     | 313 | ARG  | CB-CG-CD    | -5.45 | 98.76       | 111.30   |
| 7   | U     | 622 | SER  | N-CA-C      | -5.34 | 107.42      | 114.04   |
| 5   | I     | 146 | DG   | C4'-C3'-O3' | 5.28  | 117.92      | 110.00   |
| 6   | J     | 303 | DG   | C2'-C3'-O3' | 5.28  | 119.41      | 111.50   |
| 5   | I     | 67  | DG   | C2'-C3'-O3' | -5.27 | 103.60      | 111.50   |
| 5   | I     | 144 | DC   | C2'-C3'-O3' | 5.14  | 119.22      | 111.50   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 8   | V     | 1006 | LYS  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 801   | 0        | 831      | 61      | 0            |
| 1   | E     | 779   | 0        | 815      | 61      | 0            |
| 1   | K     | 801   | 0        | 831      | 81      | 0            |
| 1   | O     | 779   | 0        | 815      | 66      | 0            |
| 2   | B     | 653   | 0        | 695      | 41      | 0            |
| 2   | F     | 672   | 0        | 698      | 71      | 0            |
| 2   | L     | 707   | 0        | 760      | 88      | 0            |
| 2   | P     | 632   | 0        | 665      | 48      | 0            |
| 3   | C     | 811   | 0        | 849      | 75      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | G     | 815   | 0        | 860      | 65      | 0            |
| 3   | M     | 811   | 0        | 849      | 67      | 0            |
| 3   | Q     | 815   | 0        | 860      | 57      | 0            |
| 4   | D     | 717   | 0        | 723      | 56      | 0            |
| 4   | H     | 725   | 0        | 745      | 47      | 0            |
| 4   | N     | 717   | 0        | 723      | 59      | 0            |
| 4   | R     | 725   | 0        | 745      | 55      | 0            |
| 5   | I     | 6918  | 0        | 3807     | 147     | 0            |
| 6   | J     | 6981  | 0        | 3802     | 182     | 0            |
| 7   | U     | 4840  | 0        | 4833     | 412     | 0            |
| 8   | V     | 6552  | 0        | 6584     | 479     | 0            |
| 9   | V     | 27    | 0        | 12       | 6       | 0            |
| 10  | V     | 4     | 0        | 0        | 3       | 0            |
| 11  | V     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 37283 | 0        | 31502    | 1914    | 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 (1914) 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) |
|------------------|------------------|--------------------------|-------------------|
| 6:J:284:DA:H2''  | 6:J:285:DT:C5'   | 1.72                     | 1.19              |
| 6:J:284:DA:H2''  | 6:J:285:DT:H5'   | 1.17                     | 1.14              |
| 6:J:283:DA:H2''  | 6:J:284:DA:OP2   | 1.40                     | 1.11              |
| 8:V:364:TRP:HA   | 8:V:367:LEU:HB3  | 1.46                     | 0.97              |
| 2:L:29:ILE:HD11  | 2:L:55:ARG:HG2   | 1.47                     | 0.94              |
| 7:U:325:ILE:O    | 7:U:358:ASN:ND2  | 2.00                     | 0.94              |
| 2:F:78:ARG:HE    | 2:F:79:LYS:H     | 0.98                     | 0.92              |
| 6:J:284:DA:C2'   | 6:J:285:DT:C5'   | 2.48                     | 0.92              |
| 8:V:808:GLN:HB2  | 8:V:810:GLN:HE21 | 1.33                     | 0.91              |
| 3:Q:71:ARG:NH2   | 3:Q:75:LYS:O     | 2.05                     | 0.89              |
| 2:F:52:GLU:OE1   | 2:F:55:ARG:NH1   | 2.06                     | 0.88              |
| 5:I:263:DC:N3    | 6:J:52:DG:N1     | 2.21                     | 0.87              |
| 3:M:30:VAL:HG11  | 3:M:51:LEU:HD11  | 1.55                     | 0.87              |
| 8:V:418:GLU:HB3  | 8:V:421:LEU:H    | 1.40                     | 0.86              |
| 1:O:57:SER:OG    | 2:P:40:ARG:NH2   | 2.08                     | 0.86              |
| 8:V:338:GLN:HA   | 8:V:341:ARG:HE   | 1.40                     | 0.86              |
| 5:I:214:DC:H4'   | 5:I:215:DT:H5'   | 1.58                     | 0.85              |
| 6:J:284:DA:C2'   | 6:J:285:DT:H5'   | 2.03                     | 0.85              |
| 7:U:543:VAL:HG13 | 7:U:546:ILE:HB   | 1.58                     | 0.85              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:82:THR:HB    | 2:F:84:MET:HE3    | 1.60                     | 0.84              |
| 3:M:39:TYR:HB3   | 4:N:75:SER:HB2    | 1.60                     | 0.83              |
| 7:U:420:PRO:HG2  | 7:U:424:ILE:HA    | 1.61                     | 0.83              |
| 5:I:81:DC:O2     | 6:J:234:DG:N2     | 2.12                     | 0.83              |
| 8:V:827:LYS:HD2  | 8:V:864:ASN:HB3   | 1.61                     | 0.83              |
| 7:U:182:ILE:HA   | 7:U:185:LEU:HD12  | 1.62                     | 0.82              |
| 7:U:276:LYS:NZ   | 7:U:280:PRO:O     | 2.13                     | 0.82              |
| 7:U:303:ARG:NH2  | 7:U:370:LEU:O     | 2.13                     | 0.82              |
| 8:V:997:ASP:OD2  | 8:V:1045:ARG:NH2  | 2.12                     | 0.81              |
| 5:I:218:DC:N3    | 6:J:97:DG:N1      | 2.29                     | 0.81              |
| 7:U:553:ARG:NH1  | 7:U:598:SER:O     | 2.14                     | 0.81              |
| 8:V:995:GLU:HA   | 8:V:998:ARG:HG3   | 1.63                     | 0.81              |
| 7:U:226:ILE:HG13 | 7:U:236:LEU:HB2   | 1.62                     | 0.80              |
| 8:V:1025:CYS:HB3 | 8:V:1028:PHE:HB2  | 1.63                     | 0.80              |
| 6:J:283:DA:C2'   | 6:J:284:DA:OP2    | 2.28                     | 0.80              |
| 7:U:394:ALA:HB1  | 7:U:398:TRP:CZ3   | 2.15                     | 0.80              |
| 5:I:274:DC:N3    | 6:J:41:DG:N1      | 2.26                     | 0.80              |
| 8:V:107:LYS:NZ   | 8:V:212:LYS:O     | 2.15                     | 0.80              |
| 7:U:309:TRP:HB3  | 7:U:398:TRP:NE1   | 1.98                     | 0.79              |
| 3:M:54:VAL:HG22  | 4:N:107:ALA:HB1   | 1.62                     | 0.79              |
| 8:V:332:GLU:O    | 8:V:338:GLN:NE2   | 2.15                     | 0.79              |
| 7:U:191:LYS:NZ   | 7:U:533:LEU:O     | 2.16                     | 0.79              |
| 7:U:555:HIS:NE2  | 7:U:557:TYR:O     | 2.15                     | 0.79              |
| 6:J:148:DG:H2''  | 6:J:149:DT:H5'    | 1.63                     | 0.78              |
| 7:U:418:LYS:NZ   | 7:U:419:ASP:O     | 2.15                     | 0.78              |
| 1:K:127:ALA:O    | 1:K:131:ARG:N     | 2.15                     | 0.78              |
| 7:U:316:ARG:NH2  | 8:V:1020:ASP:HB3  | 1.98                     | 0.78              |
| 2:F:78:ARG:HE    | 2:F:79:LYS:N      | 1.80                     | 0.78              |
| 6:J:284:DA:H1'   | 6:J:285:DT:H5''   | 1.63                     | 0.78              |
| 2:L:63:GLU:HA    | 2:L:66:ILE:HB     | 1.66                     | 0.78              |
| 8:V:949:ASN:O    | 8:V:953:LYS:NZ    | 2.17                     | 0.78              |
| 8:V:596:TYR:HA   | 8:V:626:LEU:HD12  | 1.66                     | 0.78              |
| 8:V:1023:ARG:HA  | 8:V:1035:ARG:HH12 | 1.49                     | 0.78              |
| 7:U:575:LEU:HA   | 7:U:578:LYS:HE2   | 1.66                     | 0.78              |
| 6:J:0:DC:H2''    | 6:J:1:DT:C5       | 2.19                     | 0.77              |
| 8:V:356:LEU:HD23 | 8:V:363:LEU:HD13  | 1.65                     | 0.77              |
| 8:V:982:HIS:HB2  | 8:V:983:PRO:HD3   | 1.66                     | 0.77              |
| 7:U:214:LEU:O    | 7:U:238:TYR:OH    | 2.01                     | 0.77              |
| 1:K:122:LYS:HG3  | 1:O:113:HIS:HE1   | 1.47                     | 0.77              |
| 7:U:483:LEU:HD23 | 7:U:486:ILE:HD11  | 1.67                     | 0.77              |
| 8:V:436:MET:SD   | 8:V:439:LYS:NZ    | 2.58                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:U:486:ILE:HG21 | 7:U:508:LYS:HE2  | 1.66                     | 0.76              |
| 3:C:77:ARG:HH21  | 5:I:132:DG:H5''  | 1.50                     | 0.76              |
| 7:U:190:ASN:OD1  | 7:U:555:HIS:ND1  | 2.16                     | 0.76              |
| 1:K:113:HIS:NE2  | 1:O:123:ASP:OD1  | 2.18                     | 0.76              |
| 5:I:164:DC:H42   | 6:J:151:DG:H22   | 1.31                     | 0.76              |
| 1:K:113:HIS:HE1  | 1:O:122:LYS:HG3  | 1.49                     | 0.76              |
| 7:U:426:THR:OG1  | 7:U:427:GLN:OE1  | 2.04                     | 0.76              |
| 5:I:165:DG:N1    | 6:J:150:DC:O2    | 2.18                     | 0.76              |
| 2:L:65:VAL:O     | 2:L:69:ALA:N     | 2.17                     | 0.76              |
| 7:U:394:ALA:HB1  | 7:U:398:TRP:HZ3  | 1.51                     | 0.76              |
| 1:K:66:PRO:HA    | 1:K:69:ARG:NE    | 2.01                     | 0.76              |
| 3:C:77:ARG:HG2   | 4:D:50:GLY:HA3   | 1.68                     | 0.75              |
| 7:U:650:LYS:HG2  | 7:U:700:ARG:HD2  | 1.66                     | 0.75              |
| 2:F:39:ARG:NH1   | 2:F:43:VAL:O     | 2.18                     | 0.75              |
| 1:K:70:LEU:HD23  | 2:L:25:ASN:HB3   | 1.69                     | 0.75              |
| 1:E:54:TYR:HB3   | 2:F:40:ARG:HG2   | 1.69                     | 0.75              |
| 4:H:102:GLU:O    | 4:H:106:HIS:ND1  | 2.18                     | 0.75              |
| 1:E:109:LEU:HD13 | 1:E:112:ILE:HD11 | 1.69                     | 0.75              |
| 5:I:218:DC:O2    | 6:J:97:DG:N2     | 2.16                     | 0.75              |
| 8:V:480:TYR:HA   | 8:V:485:ALA:HB3  | 1.68                     | 0.75              |
| 4:D:37:TYR:HD1   | 4:D:40:LYS:HZ2   | 1.35                     | 0.74              |
| 2:L:20:LYS:HZ1   | 2:L:23:ARG:HD2   | 1.50                     | 0.74              |
| 1:A:59:GLU:O     | 2:B:40:ARG:NH1   | 2.17                     | 0.74              |
| 3:C:29:ARG:HG3   | 3:C:32:ARG:HH21  | 1.52                     | 0.74              |
| 7:U:346:HIS:O    | 8:V:905:ASN:ND2  | 2.21                     | 0.74              |
| 1:K:66:PRO:HA    | 1:K:69:ARG:HE    | 1.51                     | 0.74              |
| 3:C:31:HIS:CD2   | 3:C:35:ARG:HE    | 2.05                     | 0.74              |
| 1:E:61:LEU:HD12  | 2:F:37:LEU:HD23  | 1.70                     | 0.73              |
| 5:I:81:DC:N3     | 6:J:234:DG:N1    | 2.29                     | 0.73              |
| 6:J:56:DG:OP2    | 8:V:551:SER:N    | 2.20                     | 0.73              |
| 5:I:227:DA:H3'   | 1:O:63:ARG:HH21  | 1.52                     | 0.73              |
| 3:G:95:LYS:HE2   | 4:H:100:PRO:HG2  | 1.71                     | 0.73              |
| 7:U:420:PRO:HD2  | 7:U:424:ILE:HG12 | 1.71                     | 0.73              |
| 7:U:431:ARG:HH21 | 7:U:521:PRO:HB3  | 1.53                     | 0.73              |
| 8:V:443:LYS:HD3  | 8:V:460:GLU:HG2  | 1.69                     | 0.73              |
| 8:V:535:GLU:OE1  | 8:V:547:ARG:NH1  | 2.21                     | 0.73              |
| 8:V:978:LEU:HB3  | 8:V:998:ARG:HD2  | 1.71                     | 0.73              |
| 1:A:74:ILE:HD12  | 2:B:62:LEU:HD23  | 1.71                     | 0.72              |
| 3:C:80:PRO:HA    | 3:C:83:LEU:HD13  | 1.71                     | 0.72              |
| 2:L:75:HIS:CE1   | 4:N:89:ARG:HG2   | 2.25                     | 0.72              |
| 3:G:92:GLU:HB3   | 4:H:103:LEU:HD11 | 1.72                     | 0.72              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:V:613:HIS:HB2  | 8:V:621:VAL:HG21  | 1.72                     | 0.72              |
| 8:V:1054:GLU:HA  | 8:V:1061:ILE:HD11 | 1.71                     | 0.72              |
| 7:U:634:SER:HB3  | 7:U:714:TYR:HE2   | 1.55                     | 0.72              |
| 8:V:603:GLN:NE2  | 8:V:647:ASP:OD2   | 2.23                     | 0.72              |
| 1:A:43:PRO:HB2   | 6:J:236:DG:H5''   | 1.72                     | 0.72              |
| 3:Q:87:VAL:HG13  | 3:Q:93:LEU:HB3    | 1.71                     | 0.71              |
| 8:V:958:LYS:HA   | 8:V:1011:ARG:HH22 | 1.56                     | 0.71              |
| 5:I:160:DA:N6    | 6:J:155:DT:O2     | 2.23                     | 0.71              |
| 3:M:65:LEU:HD11  | 8:V:769:ARG:HH22  | 1.55                     | 0.71              |
| 3:M:78:ILE:HB    | 4:N:51:ILE:HG22   | 1.73                     | 0.71              |
| 8:V:470:MET:HE1  | 8:V:473:ARG:HH21  | 1.56                     | 0.71              |
| 8:V:607:GLN:O    | 8:V:611:ARG:NH2   | 2.22                     | 0.71              |
| 8:V:902:TYR:O    | 8:V:906:SER:OG    | 2.08                     | 0.71              |
| 5:I:150:DC:H5'   | 6:J:168:DT:H4'    | 1.73                     | 0.71              |
| 2:F:63:GLU:HA    | 2:F:66:ILE:HG22   | 1.73                     | 0.71              |
| 4:H:99:LEU:HD23  | 4:H:103:LEU:HB3   | 1.71                     | 0.71              |
| 6:J:-4:DT:H2''   | 6:J:-3:DA:C8      | 2.26                     | 0.71              |
| 7:U:613:HIS:HB3  | 7:U:617:ARG:HE    | 1.54                     | 0.71              |
| 4:N:74:ALA:HA    | 4:N:77:LEU:HD12   | 1.72                     | 0.71              |
| 3:Q:77:ARG:HG2   | 4:R:50:GLY:HA3    | 1.71                     | 0.71              |
| 8:V:319:GLU:OE1  | 8:V:346:ARG:NE    | 2.20                     | 0.71              |
| 4:D:30:ARG:HE    | 5:I:123:DC:H4'    | 1.56                     | 0.71              |
| 7:U:327:LYS:HB2  | 7:U:328:PRO:HD3   | 1.73                     | 0.71              |
| 7:U:576:LEU:HD13 | 7:U:712:ASP:HB3   | 1.73                     | 0.71              |
| 2:L:75:HIS:HE1   | 4:N:89:ARG:HG2    | 1.56                     | 0.71              |
| 7:U:437:VAL:HG23 | 7:U:569:LEU:HD21  | 1.70                     | 0.70              |
| 1:K:129:ARG:NH1  | 1:K:129:ARG:O     | 2.23                     | 0.70              |
| 6:J:120:DG:H4'   | 6:J:121:DA:H5'    | 1.72                     | 0.70              |
| 7:U:554:LEU:HD13 | 7:U:598:SER:H     | 1.54                     | 0.70              |
| 3:G:52:ALA:HA    | 3:G:55:LEU:HD12   | 1.72                     | 0.70              |
| 3:Q:52:ALA:HA    | 3:Q:55:LEU:HD12   | 1.72                     | 0.70              |
| 1:E:79:LYS:HB3   | 1:E:82:LEU:HD11   | 1.71                     | 0.70              |
| 5:I:214:DC:N3    | 6:J:100:DA:N6     | 2.39                     | 0.70              |
| 3:M:97:LEU:HD12  | 3:M:100:VAL:HG11  | 1.73                     | 0.70              |
| 1:E:51:ILE:HD12  | 2:F:42:GLY:HA2    | 1.72                     | 0.70              |
| 7:U:374:GLU:OE1  | 7:U:374:GLU:N     | 2.24                     | 0.70              |
| 5:I:270:DA:H2'   | 5:I:271:DT:H71    | 1.73                     | 0.70              |
| 8:V:958:LYS:HG3  | 8:V:1011:ARG:HH12 | 1.56                     | 0.70              |
| 1:E:100:LEU:HA   | 1:E:103:LEU:HD12  | 1.72                     | 0.69              |
| 8:V:503:LYS:NZ   | 8:V:596:TYR:O     | 2.22                     | 0.69              |
| 7:U:193:SER:HB2  | 7:U:555:HIS:CE1   | 2.28                     | 0.69              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:U:590:PHE:HA   | 7:U:594:GLY:HA3   | 1.72                     | 0.69              |
| 8:V:821:GLU:OE2  | 8:V:876:LYS:NZ    | 2.25                     | 0.69              |
| 7:U:226:ILE:O    | 7:U:236:LEU:N     | 2.24                     | 0.69              |
| 7:U:335:GLN:OE1  | 8:V:912:ARG:NH1   | 2.25                     | 0.69              |
| 8:V:1039:PRO:HA  | 8:V:1042:LEU:HB2  | 1.73                     | 0.69              |
| 1:E:47:ALA:O     | 1:E:51:ILE:HG12   | 1.92                     | 0.69              |
| 6:J:284:DA:C2'   | 6:J:285:DT:H5''   | 2.22                     | 0.69              |
| 2:B:29:ILE:O     | 2:B:55:ARG:NH2    | 2.19                     | 0.69              |
| 3:G:76:THR:O     | 4:H:50:GLY:N      | 2.22                     | 0.69              |
| 8:V:975:PHE:O    | 8:V:998:ARG:NH2   | 2.23                     | 0.69              |
| 1:E:89:VAL:HA    | 1:E:92:LEU:HD12   | 1.74                     | 0.69              |
| 2:F:47:SER:HB3   | 2:F:50:ILE:HG12   | 1.72                     | 0.69              |
| 3:M:41:GLU:OE2   | 4:N:84:SER:HB2    | 1.93                     | 0.69              |
| 8:V:1000:ILE:O   | 8:V:1004:LEU:N    | 2.23                     | 0.69              |
| 7:U:348:GLU:O    | 8:V:905:ASN:ND2   | 2.24                     | 0.69              |
| 8:V:279:ASP:H    | 8:V:282:GLU:HB2   | 1.57                     | 0.69              |
| 8:V:377:ASP:HB3  | 8:V:380:ASP:HB2   | 1.73                     | 0.69              |
| 8:V:959:MET:HA   | 8:V:962:GLU:HB3   | 1.75                     | 0.69              |
| 5:I:217:DG:N2    | 6:J:99:DT:O2      | 2.26                     | 0.69              |
| 7:U:350:LEU:HG   | 8:V:958:LYS:HE3   | 1.75                     | 0.69              |
| 2:B:23:ARG:HH12  | 7:U:248:VAL:HG13  | 1.58                     | 0.68              |
| 7:U:553:ARG:NH1  | 7:U:598:SER:OG    | 2.25                     | 0.68              |
| 1:A:90:MET:O     | 1:A:93:GLN:HG3    | 1.94                     | 0.68              |
| 1:K:76:GLN:HE22  | 1:K:80:THR:HG22   | 1.57                     | 0.68              |
| 3:M:95:LYS:HZ1   | 4:N:100:PRO:HG3   | 1.57                     | 0.68              |
| 8:V:975:PHE:HB2  | 8:V:1002:LEU:HD11 | 1.76                     | 0.68              |
| 2:L:56:GLY:HA2   | 2:L:59:LYS:HE3    | 1.75                     | 0.68              |
| 8:V:107:LYS:HD2  | 8:V:214:LYS:HD2   | 1.74                     | 0.68              |
| 8:V:1031:ASP:OD1 | 8:V:1032:PHE:N    | 2.27                     | 0.68              |
| 7:U:538:PHE:CG   | 7:U:552:PRO:HA    | 2.28                     | 0.68              |
| 7:U:656:LYS:HG3  | 7:U:657:GLU:HG2   | 1.74                     | 0.68              |
| 8:V:104:GLY:O    | 8:V:108:ARG:N     | 2.22                     | 0.68              |
| 4:R:66:VAL:HA    | 4:R:69:ARG:HG2    | 1.74                     | 0.68              |
| 2:L:58:LEU:O     | 2:L:62:LEU:HG     | 1.94                     | 0.67              |
| 8:V:237:TYR:HD2  | 8:V:238:LEU:HD22  | 1.59                     | 0.67              |
| 8:V:371:LEU:HB3  | 8:V:374:ILE:HD12  | 1.74                     | 0.67              |
| 8:V:520:ARG:HH12 | 8:V:569:SER:HB3   | 1.59                     | 0.67              |
| 1:E:62:ILE:HB    | 1:E:93:GLN:HE21   | 1.59                     | 0.67              |
| 3:G:96:LEU:HD11  | 4:H:103:LEU:HD13  | 1.76                     | 0.67              |
| 6:J:7:DT:H2''    | 6:J:8:DG:C8       | 2.29                     | 0.67              |
| 7:U:317:GLN:N    | 7:U:361:GLU:O     | 2.27                     | 0.67              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:55:ALA:HA    | 4:D:58:ILE:HD12   | 1.74                     | 0.67              |
| 5:I:131:DA:H1'   | 5:I:132:DG:C8     | 2.30                     | 0.67              |
| 5:I:217:DG:H4'   | 1:O:83:ARG:HD3    | 1.77                     | 0.67              |
| 8:V:834:THR:H    | 8:V:837:ASP:HB2   | 1.58                     | 0.67              |
| 8:V:839:LYS:HA   | 8:V:842:TYR:HB2   | 1.76                     | 0.67              |
| 3:C:57:TYR:HB2   | 4:D:110:GLU:OE1   | 1.95                     | 0.67              |
| 3:G:90:ASP:OD2   | 3:G:93:LEU:N      | 2.18                     | 0.67              |
| 7:U:647:LYS:O    | 7:U:700:ARG:NH1   | 2.26                     | 0.67              |
| 3:C:88:ARG:NH1   | 3:C:94:ASN:OD1    | 2.27                     | 0.67              |
| 3:G:92:GLU:HA    | 3:G:95:LYS:HZ2    | 1.60                     | 0.67              |
| 5:I:159:DA:H2'   | 5:I:160:DA:C8     | 2.30                     | 0.67              |
| 3:Q:88:ARG:NH2   | 3:Q:100:VAL:O     | 2.28                     | 0.67              |
| 7:U:428:GLN:HE22 | 7:U:534:ARG:HB2   | 1.58                     | 0.67              |
| 4:R:94:ALA:O     | 4:R:98:LEU:N      | 2.27                     | 0.67              |
| 8:V:832:VAL:HG13 | 8:V:858:LEU:HG    | 1.77                     | 0.67              |
| 7:U:648:ILE:HG12 | 7:U:703:LEU:HB3   | 1.76                     | 0.67              |
| 3:C:90:ASP:OD2   | 3:C:93:LEU:N      | 2.19                     | 0.66              |
| 5:I:174:DA:H2''  | 5:I:175:DA:H8     | 1.61                     | 0.66              |
| 7:U:334:GLU:HG2  | 7:U:353:ASN:HA    | 1.77                     | 0.66              |
| 3:G:102:ILE:HG23 | 3:G:105:GLY:HA3   | 1.77                     | 0.66              |
| 8:V:564:TYR:CE1  | 8:V:574:PHE:HB2   | 2.31                     | 0.66              |
| 8:V:911:ALA:HA   | 8:V:914:LEU:HB2   | 1.75                     | 0.66              |
| 8:V:887:TRP:NE1  | 8:V:922:GLU:OE2   | 2.15                     | 0.66              |
| 8:V:1014:VAL:HA  | 8:V:1017:LEU:HD12 | 1.77                     | 0.66              |
| 1:A:113:HIS:HE1  | 1:E:122:LYS:HB3   | 1.59                     | 0.66              |
| 6:J:83:DT:H5'    | 1:O:43:PRO:HA     | 1.77                     | 0.66              |
| 7:U:325:ILE:HB   | 7:U:328:PRO:HD2   | 1.76                     | 0.66              |
| 1:K:84:PHE:HA    | 2:L:81:VAL:HG22   | 1.76                     | 0.66              |
| 8:V:218:ILE:HG12 | 8:V:350:LEU:HB3   | 1.77                     | 0.66              |
| 8:V:399:LYS:HE2  | 8:V:402:HIS:HD2   | 1.61                     | 0.66              |
| 7:U:619:ARG:NH2  | 7:U:622:SER:OG    | 2.28                     | 0.66              |
| 4:N:99:LEU:HD23  | 4:N:104:ALA:HA    | 1.77                     | 0.66              |
| 3:Q:46:GLY:O     | 3:Q:50:TYR:N      | 2.23                     | 0.66              |
| 7:U:151:ILE:HD11 | 7:U:525:PRO:HB3   | 1.77                     | 0.66              |
| 7:U:690:LEU:HB2  | 7:U:700:ARG:HH22  | 1.60                     | 0.66              |
| 5:I:274:DC:N4    | 6:J:41:DG:O6      | 2.27                     | 0.66              |
| 8:V:968:LEU:HD13 | 8:V:1005:PHE:HD1  | 1.61                     | 0.66              |
| 4:D:66:VAL:O     | 4:D:70:ILE:HG12   | 1.96                     | 0.66              |
| 4:H:87:THR:N     | 4:H:90:GLU:OE2    | 2.25                     | 0.66              |
| 6:J:284:DA:C1'   | 6:J:285:DT:H5''   | 2.25                     | 0.66              |
| 7:U:555:HIS:CE1  | 7:U:557:TYR:HB2   | 2.31                     | 0.66              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:U:349:ILE:HG13 | 7:U:351:THR:H     | 1.60                     | 0.65              |
| 7:U:383:LEU:O    | 7:U:388:ARG:NH1   | 2.28                     | 0.65              |
| 3:C:52:ALA:HA    | 3:C:55:LEU:HD12   | 1.78                     | 0.65              |
| 8:V:823:MET:HE1  | 8:V:860:LEU:HG    | 1.79                     | 0.65              |
| 8:V:888:ASN:O    | 8:V:892:PHE:N     | 2.23                     | 0.65              |
| 8:V:822:ARG:HH22 | 8:V:833:PRO:HG3   | 1.59                     | 0.65              |
| 2:F:30:THR:HG21  | 5:I:61:DA:H5''    | 1.78                     | 0.65              |
| 7:U:228:LYS:HD3  | 7:U:236:LEU:HD11  | 1.78                     | 0.65              |
| 8:V:934:ILE:HD12 | 8:V:937:ILE:HD12  | 1.77                     | 0.65              |
| 8:V:1005:PHE:C   | 8:V:1008:GLY:H    | 2.04                     | 0.65              |
| 3:G:64:GLU:OE2   | 3:G:68:ASN:ND2    | 2.29                     | 0.65              |
| 1:O:64:LYS:O     | 1:O:68:GLN:N      | 2.24                     | 0.65              |
| 7:U:393:ARG:O    | 7:U:396:THR:OG1   | 2.14                     | 0.65              |
| 3:G:29:ARG:HG3   | 3:G:32:ARG:HH21   | 1.62                     | 0.65              |
| 7:U:199:ASP:OD2  | 7:U:284:TRP:NE1   | 2.18                     | 0.65              |
| 8:V:994:GLU:HG2  | 8:V:998:ARG:HH11  | 1.62                     | 0.65              |
| 8:V:1015:TYR:CE2 | 8:V:1043:ALA:HA   | 2.32                     | 0.65              |
| 2:F:48:GLY:HA2   | 2:F:51:TYR:CE2    | 2.32                     | 0.65              |
| 7:U:486:ILE:O    | 7:U:490:LEU:HB2   | 1.97                     | 0.65              |
| 2:L:63:GLU:O     | 2:L:67:ARG:N      | 2.23                     | 0.65              |
| 3:M:52:ALA:HA    | 3:M:55:LEU:HD12   | 1.79                     | 0.65              |
| 8:V:1001:LEU:HA  | 8:V:1004:LEU:HD12 | 1.79                     | 0.65              |
| 4:H:43:LYS:HE3   | 4:H:47:PRO:HA     | 1.78                     | 0.64              |
| 5:I:276:DC:H2''  | 5:I:277:DC:C5     | 2.31                     | 0.64              |
| 6:J:146:DA:H1'   | 6:J:147:DG:H5'    | 1.78                     | 0.64              |
| 7:U:520:GLN:HB2  | 7:U:523:ALA:HB2   | 1.78                     | 0.64              |
| 8:V:313:LEU:HD22 | 8:V:318:TRP:HZ2   | 1.61                     | 0.64              |
| 3:G:29:ARG:HD2   | 4:H:32:GLU:OE2    | 1.97                     | 0.64              |
| 7:U:585:ASN:N    | 7:U:588:THR:OG1   | 2.29                     | 0.64              |
| 3:M:41:GLU:HG2   | 3:M:42:ARG:HG3    | 1.79                     | 0.64              |
| 8:V:894:LYS:HE2  | 8:V:914:LEU:HD23  | 1.78                     | 0.64              |
| 8:V:1019:ARG:HG3 | 8:V:1039:PRO:HD3  | 1.78                     | 0.64              |
| 3:G:41:GLU:OE1   | 3:G:42:ARG:HG3    | 1.97                     | 0.64              |
| 1:K:131:ARG:HH22 | 1:O:131:ARG:HD3   | 1.62                     | 0.64              |
| 8:V:357:GLN:N    | 8:V:362:GLU:OE2   | 2.23                     | 0.64              |
| 5:I:318:DT:H2''  | 5:I:319:DA:C8     | 2.32                     | 0.64              |
| 7:U:150:VAL:HB   | 7:U:523:ALA:H     | 1.63                     | 0.64              |
| 8:V:320:TYR:CD2  | 8:V:347:ASN:HB2   | 2.32                     | 0.64              |
| 2:F:94:GLY:O     | 2:F:95:ARG:NH2    | 2.31                     | 0.64              |
| 1:A:70:LEU:HD11  | 2:B:26:ILE:HA     | 1.80                     | 0.64              |
| 1:K:106:ASP:HA   | 1:K:109:LEU:HD12  | 1.80                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:61:LEU:HD12  | 2:B:37:LEU:HD13  | 1.79                     | 0.64              |
| 7:U:650:LYS:HE2  | 7:U:697:ASN:HA   | 1.80                     | 0.64              |
| 8:V:480:TYR:OH   | 8:V:500:ASN:OD1  | 2.16                     | 0.64              |
| 3:G:29:ARG:NH2   | 4:H:34:TYR:HD1   | 1.95                     | 0.64              |
| 6:J:2:DC:C2      | 6:J:3:DA:N7      | 2.66                     | 0.64              |
| 7:U:148:THR:OG1  | 7:U:431:ARG:NH1  | 2.31                     | 0.64              |
| 7:U:553:ARG:O    | 7:U:598:SER:OG   | 2.14                     | 0.64              |
| 8:V:962:GLU:OE2  | 8:V:965:ARG:NH2  | 2.31                     | 0.64              |
| 3:C:81:ARG:HD3   | 1:E:58:THR:HG21  | 1.81                     | 0.63              |
| 3:G:29:ARG:HH22  | 4:H:34:TYR:HA    | 1.64                     | 0.63              |
| 6:J:3:DA:H2''    | 6:J:4:DG:C8      | 2.33                     | 0.63              |
| 1:K:117:VAL:HB   | 2:L:44:LYS:HD3   | 1.80                     | 0.63              |
| 8:V:934:ILE:HA   | 8:V:937:ILE:HD12 | 1.80                     | 0.63              |
| 2:B:30:THR:HB    | 2:B:32:PRO:HD2   | 1.79                     | 0.63              |
| 2:F:78:ARG:NE    | 2:F:79:LYS:H     | 1.82                     | 0.63              |
| 5:I:263:DC:N4    | 6:J:52:DG:O6     | 2.31                     | 0.63              |
| 3:M:65:LEU:HD11  | 8:V:769:ARG:NH2  | 2.13                     | 0.63              |
| 8:V:249:LEU:HD22 | 8:V:321:ILE:HG23 | 1.80                     | 0.63              |
| 8:V:592:VAL:HG12 | 8:V:622:LYS:HB2  | 1.78                     | 0.63              |
| 7:U:578:LYS:HG2  | 7:U:584:TYR:HE2  | 1.64                     | 0.63              |
| 2:L:90:LEU:HA    | 2:L:93:GLN:NE2   | 2.13                     | 0.63              |
| 8:V:808:GLN:OE1  | 8:V:810:GLN:NE2  | 2.31                     | 0.63              |
| 3:G:44:GLY:HA2   | 6:J:279:DG:H5''  | 1.81                     | 0.63              |
| 7:U:585:ASN:O    | 7:U:589:LEU:N    | 2.31                     | 0.63              |
| 8:V:1021:GLU:O   | 8:V:1025:CYS:N   | 2.32                     | 0.63              |
| 7:U:445:LYS:HE2  | 7:U:499:ASP:HA   | 1.81                     | 0.63              |
| 8:V:520:ARG:NE   | 8:V:571:LYS:O    | 2.31                     | 0.63              |
| 8:V:893:ARG:NH2  | 8:V:943:TYR:OH   | 2.32                     | 0.63              |
| 8:V:1003:MET:HE2 | 8:V:1021:GLU:HG3 | 1.81                     | 0.63              |
| 2:F:91:LYS:NZ    | 4:H:76:ARG:HH12  | 1.97                     | 0.63              |
| 1:K:86:SER:O     | 1:K:90:MET:N     | 2.22                     | 0.63              |
| 1:O:95:ALA:O     | 2:P:95:ARG:NH2   | 2.32                     | 0.63              |
| 5:I:123:DC:H2''  | 5:I:124:DA:C8    | 2.33                     | 0.63              |
| 1:K:69:ARG:NH1   | 2:L:25:ASN:OD1   | 2.31                     | 0.63              |
| 7:U:697:ASN:OD1  | 7:U:698:THR:N    | 2.29                     | 0.62              |
| 7:U:381:LEU:C    | 7:U:388:ARG:HH21 | 2.07                     | 0.62              |
| 7:U:459:SER:HB2  | 7:U:480:LEU:HD22 | 1.81                     | 0.62              |
| 3:G:85:LEU:O     | 3:G:89:ASN:ND2   | 2.32                     | 0.62              |
| 6:J:-7:DG:H1'    | 6:J:-6:DA:H5'    | 1.82                     | 0.62              |
| 7:U:333:PHE:H    | 7:U:355:TYR:HA   | 1.64                     | 0.62              |
| 7:U:426:THR:HA   | 7:U:534:ARG:HD2  | 1.81                     | 0.62              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:U:430:PRO:HG3   | 7:U:525:PRO:HG2  | 1.82                     | 0.62              |
| 4:N:73:GLU:O      | 4:N:77:LEU:HG    | 1.99                     | 0.62              |
| 8:V:1019:ARG:HH11 | 8:V:1023:ARG:HE  | 1.45                     | 0.62              |
| 8:V:1023:ARG:HA   | 8:V:1035:ARG:NH1 | 2.13                     | 0.62              |
| 3:C:45:ALA:O      | 3:C:48:PRO:HD2   | 1.99                     | 0.62              |
| 5:I:182:DT:H2''   | 5:I:183:DG:C8    | 2.35                     | 0.62              |
| 7:U:162:TYR:HD1   | 7:U:613:HIS:CE1  | 2.18                     | 0.62              |
| 1:O:61:LEU:HD12   | 2:P:37:LEU:HD23  | 1.81                     | 0.62              |
| 8:V:504:LEU:HA    | 8:V:507:LEU:HB2  | 1.81                     | 0.62              |
| 8:V:959:MET:O     | 8:V:963:ALA:N    | 2.32                     | 0.62              |
| 3:C:91:GLU:HG2    | 3:C:92:GLU:N     | 2.14                     | 0.62              |
| 7:U:316:ARG:HH22  | 8:V:1020:ASP:HB3 | 1.63                     | 0.62              |
| 1:K:62:ILE:HD11   | 2:L:37:LEU:HD11  | 1.81                     | 0.62              |
| 3:M:61:GLU:HG3    | 8:V:769:ARG:NH1  | 2.13                     | 0.62              |
| 1:A:120:MET:HE3   | 1:A:121:PRO:HD2  | 1.80                     | 0.62              |
| 7:U:185:LEU:O     | 7:U:189:ILE:HG12 | 1.98                     | 0.62              |
| 3:C:25:PHE:N      | 3:C:56:GLU:OE2   | 2.33                     | 0.62              |
| 6:J:41:DG:H2'     | 6:J:42:DT:H71    | 1.82                     | 0.62              |
| 1:K:57:SER:OG     | 2:L:40:ARG:NH2   | 2.28                     | 0.62              |
| 1:K:122:LYS:O     | 1:K:125:GLN:NE2  | 2.30                     | 0.62              |
| 3:C:92:GLU:OE1    | 4:D:103:LEU:HG   | 2.00                     | 0.62              |
| 5:I:184:DC:H2''   | 5:I:185:DC:C5    | 2.35                     | 0.62              |
| 7:U:309:TRP:HB3   | 7:U:398:TRP:CD1  | 2.35                     | 0.62              |
| 7:U:682:ASN:ND2   | 7:U:689:PRO:HD3  | 2.14                     | 0.62              |
| 3:Q:16:THR:O      | 3:Q:19:SER:OG    | 2.16                     | 0.62              |
| 8:V:188:SER:HB2   | 8:V:201:ILE:HD11 | 1.80                     | 0.62              |
| 8:V:291:LEU:HD11  | 8:V:299:VAL:HG21 | 1.81                     | 0.62              |
| 3:C:28:GLY:HA3    | 6:J:197:DG:H3'   | 1.81                     | 0.62              |
| 7:U:212:LEU:HD21  | 7:U:254:MET:HG2  | 1.81                     | 0.62              |
| 7:U:634:SER:HB3   | 7:U:714:TYR:CE2  | 2.35                     | 0.62              |
| 1:K:69:ARG:HH12   | 2:L:25:ASN:HA    | 1.65                     | 0.62              |
| 2:L:59:LYS:O      | 2:L:62:LEU:N     | 2.32                     | 0.62              |
| 4:H:87:THR:OG1    | 4:H:90:GLU:OE1   | 2.14                     | 0.62              |
| 7:U:613:HIS:O     | 7:U:617:ARG:HB2  | 2.00                     | 0.62              |
| 5:I:172:DA:H2''   | 5:I:173:DG:C8    | 2.35                     | 0.61              |
| 2:L:93:GLN:O      | 2:L:95:ARG:NH1   | 2.33                     | 0.61              |
| 1:O:83:ARG:O      | 2:P:81:VAL:N     | 2.30                     | 0.61              |
| 3:G:92:GLU:HA     | 3:G:95:LYS:NZ    | 2.15                     | 0.61              |
| 8:V:223:MET:HE1   | 8:V:607:GLN:HA   | 1.81                     | 0.61              |
| 7:U:327:LYS:HD2   | 8:V:1006:LYS:HD3 | 1.81                     | 0.61              |
| 1:K:86:SER:HA     | 1:K:89:VAL:HB    | 1.82                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:R:65:ASP:OD2   | 4:R:69:ARG:NH2    | 2.28                     | 0.61              |
| 8:V:260:TRP:HZ3  | 8:V:324:ASP:HB2   | 1.65                     | 0.61              |
| 8:V:109:PHE:HA   | 8:V:112:LEU:HB2   | 1.83                     | 0.61              |
| 8:V:997:ASP:O    | 8:V:1000:ILE:HG12 | 2.00                     | 0.61              |
| 7:U:430:PRO:O    | 7:U:433:THR:OG1   | 2.15                     | 0.61              |
| 8:V:834:THR:O    | 8:V:838:VAL:N     | 2.28                     | 0.61              |
| 8:V:966:ARG:NH2  | 8:V:1061:ILE:O    | 2.33                     | 0.61              |
| 2:F:51:TYR:O     | 2:F:54:THR:OG1    | 2.17                     | 0.61              |
| 7:U:381:LEU:HA   | 7:U:388:ARG:HE    | 1.64                     | 0.61              |
| 4:N:76:ARG:NH1   | 4:N:80:TYR:OH     | 2.34                     | 0.61              |
| 7:U:154:LEU:HD11 | 7:U:429:VAL:HG13  | 1.82                     | 0.61              |
| 7:U:334:GLU:HB2  | 7:U:354:ILE:H     | 1.64                     | 0.61              |
| 1:K:52:ARG:HB3   | 1:K:56:LYS:HZ1    | 1.66                     | 0.61              |
| 8:V:481:LEU:HD11 | 8:V:530:LEU:HD12  | 1.82                     | 0.61              |
| 7:U:159:LYS:HG3  | 7:U:609:PRO:HG3   | 1.82                     | 0.61              |
| 3:M:115:LEU:HB3  | 2:P:44:LYS:HD2    | 1.83                     | 0.61              |
| 3:Q:41:GLU:CD    | 3:Q:42:ARG:HG3    | 2.25                     | 0.61              |
| 3:C:23:LEU:HD21  | 3:C:52:ALA:HB3    | 1.82                     | 0.60              |
| 7:U:215:TYR:H    | 7:U:222:SER:HG    | 1.49                     | 0.60              |
| 7:U:263:ASP:O    | 7:U:267:THR:N     | 2.30                     | 0.60              |
| 7:U:603:LEU:HG   | 7:U:630:LEU:HD12  | 1.83                     | 0.60              |
| 8:V:833:PRO:HD2  | 8:V:858:LEU:HA    | 1.82                     | 0.60              |
| 1:A:117:VAL:HB   | 2:B:44:LYS:HD2    | 1.83                     | 0.60              |
| 3:C:18:SER:O     | 3:C:23:LEU:N      | 2.33                     | 0.60              |
| 7:U:150:VAL:O    | 7:U:431:ARG:N     | 2.34                     | 0.60              |
| 7:U:602:LYS:HA   | 7:U:632:HIS:HA    | 1.83                     | 0.60              |
| 8:V:896:ILE:HG13 | 8:V:947:ILE:HD11  | 1.84                     | 0.60              |
| 7:U:310:GLY:O    | 7:U:398:TRP:HZ2   | 1.84                     | 0.60              |
| 7:U:327:LYS:HZ2  | 8:V:1007:TYR:N    | 2.00                     | 0.60              |
| 8:V:590:ALA:O    | 8:V:617:GLN:NE2   | 2.18                     | 0.60              |
| 2:F:75:HIS:HB2   | 4:H:93:THR:HG21   | 1.83                     | 0.60              |
| 7:U:312:PRO:O    | 7:U:316:ARG:HG3   | 2.01                     | 0.60              |
| 3:G:31:HIS:HD2   | 3:G:35:ARG:HH11   | 1.49                     | 0.60              |
| 6:J:-14:DT:OP2   | 6:J:-14:DT:H2'    | 2.02                     | 0.60              |
| 7:U:351:THR:HG21 | 8:V:909:ALA:HB2   | 1.84                     | 0.60              |
| 7:U:445:LYS:NZ   | 7:U:498:LYS:O     | 2.33                     | 0.60              |
| 2:P:78:ARG:NH1   | 2:P:80:THR:O      | 2.34                     | 0.60              |
| 3:Q:90:ASP:OD2   | 3:Q:93:LEU:N      | 2.23                     | 0.60              |
| 8:V:800:LYS:HG2  | 8:V:839:LYS:HE3   | 1.83                     | 0.60              |
| 8:V:889:LYS:HA   | 8:V:892:PHE:HB3   | 1.82                     | 0.60              |
| 7:U:461:LYS:O    | 7:U:465:VAL:N     | 2.26                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:61:LEU:HD22  | 2:P:36:ARG:HD2   | 1.84                     | 0.60              |
| 8:V:967:LYS:HD2  | 8:V:971:TYR:HD2  | 1.67                     | 0.60              |
| 7:U:679:THR:H    | 7:U:682:ASN:HD21 | 1.50                     | 0.60              |
| 3:M:62:ILE:HD11  | 4:N:59:MET:HE1   | 1.83                     | 0.60              |
| 8:V:320:TYR:HD2  | 8:V:347:ASN:HB2  | 1.65                     | 0.60              |
| 8:V:522:LEU:HB2  | 8:V:593:VAL:HG22 | 1.84                     | 0.60              |
| 8:V:1010:ASP:OD2 | 8:V:1012:ASP:HB3 | 2.01                     | 0.60              |
| 2:B:70:VAL:O     | 2:B:73:THR:N     | 2.35                     | 0.60              |
| 7:U:411:TYR:HE1  | 8:V:1033:TYR:CD1 | 2.19                     | 0.60              |
| 7:U:540:LEU:N    | 7:U:549:PHE:O    | 2.33                     | 0.60              |
| 8:V:364:TRP:NE1  | 8:V:382:ASP:OD1  | 2.35                     | 0.60              |
| 1:E:61:LEU:HD11  | 2:F:40:ARG:HD2   | 1.83                     | 0.60              |
| 8:V:814:LEU:HB2  | 8:V:879:TRP:HB3  | 1.82                     | 0.60              |
| 1:K:131:ARG:NH1  | 1:K:131:ARG:HA   | 2.16                     | 0.59              |
| 3:C:41:GLU:OE2   | 4:D:84:SER:HB2   | 2.01                     | 0.59              |
| 3:C:41:GLU:HG2   | 3:C:42:ARG:HG3   | 1.84                     | 0.59              |
| 3:M:17:ARG:HH21  | 3:M:28:GLY:HA2   | 1.67                     | 0.59              |
| 8:V:524:PHE:HB2  | 8:V:595:LEU:HD23 | 1.85                     | 0.59              |
| 8:V:896:ILE:HD13 | 8:V:943:TYR:HB3  | 1.84                     | 0.59              |
| 1:O:79:LYS:HD2   | 1:O:80:THR:H     | 1.67                     | 0.59              |
| 3:Q:30:VAL:O     | 3:Q:34:LEU:N     | 2.26                     | 0.59              |
| 8:V:433:MET:HE1  | 8:V:438:LYS:HG2  | 1.85                     | 0.59              |
| 5:I:165:DG:H5'   | 5:I:165:DG:C8    | 2.38                     | 0.59              |
| 1:K:66:PRO:O     | 1:K:70:LEU:HG    | 2.03                     | 0.59              |
| 1:O:73:GLU:OE1   | 2:P:23:ARG:N     | 2.36                     | 0.59              |
| 8:V:834:THR:HA   | 8:V:854:LYS:HE2  | 1.83                     | 0.59              |
| 8:V:934:ILE:HG13 | 8:V:940:TYR:HB2  | 1.85                     | 0.59              |
| 8:V:1062:VAL:HA  | 8:V:1065:ASP:HB3 | 1.83                     | 0.59              |
| 7:U:329:LYS:HB2  | 7:U:355:TYR:CD1  | 2.37                     | 0.59              |
| 8:V:331:ASN:HB3  | 8:V:334:SER:HB3  | 1.83                     | 0.59              |
| 8:V:833:PRO:HB3  | 8:V:857:LEU:HD23 | 1.83                     | 0.59              |
| 7:U:648:ILE:HD13 | 7:U:704:GLN:HA   | 1.84                     | 0.59              |
| 1:K:67:PHE:CE1   | 1:K:93:GLN:HB2   | 2.37                     | 0.59              |
| 2:L:50:ILE:O     | 2:L:54:THR:HG23  | 2.03                     | 0.59              |
| 1:O:99:TYR:HA    | 2:P:95:ARG:HH12  | 1.68                     | 0.59              |
| 3:Q:54:VAL:HG13  | 4:R:107:ALA:HB1  | 1.83                     | 0.59              |
| 8:V:478:HIS:NE2  | 8:V:480:TYR:HB2  | 2.18                     | 0.59              |
| 9:V:1201:ADP:O2B | 10:V:1202:BEF:F3 | 2.11                     | 0.59              |
| 7:U:262:LEU:HD13 | 7:U:298:PRO:HB2  | 1.84                     | 0.59              |
| 7:U:343:ASP:HB2  | 8:V:931:TRP:CH2  | 2.38                     | 0.59              |
| 7:U:374:GLU:O    | 7:U:378:ASN:N    | 2.35                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:V:185:PHE:O    | 8:V:205:ASN:ND2  | 2.28                     | 0.59              |
| 8:V:361:HIS:HA   | 8:V:364:TRP:NE1  | 2.18                     | 0.59              |
| 3:C:42:ARG:NE    | 4:D:85:THR:OG1   | 2.27                     | 0.59              |
| 5:I:309:DT:H2''  | 5:I:310:DC:C5    | 2.38                     | 0.59              |
| 7:U:170:ASN:HD21 | 7:U:172:ASN:HB2  | 1.68                     | 0.59              |
| 8:V:992:TYR:HB2  | 8:V:1045:ARG:NH2 | 2.17                     | 0.59              |
| 4:D:102:GLU:OE2  | 4:D:105:LYS:NZ   | 2.36                     | 0.59              |
| 6:J:61:DA:OP1    | 2:L:36:ARG:NH1   | 2.36                     | 0.59              |
| 6:J:134:DC:H2''  | 6:J:135:DC:H5'   | 1.85                     | 0.59              |
| 7:U:238:TYR:HB2  | 7:U:239:PRO:HD3  | 1.85                     | 0.59              |
| 4:N:83:ARG:HH11  | 4:N:83:ARG:HG2   | 1.68                     | 0.59              |
| 8:V:801:PRO:HD2  | 8:V:815:LYS:HE2  | 1.85                     | 0.59              |
| 1:A:48:LEU:HD23  | 1:A:52:ARG:HH22  | 1.68                     | 0.58              |
| 3:G:88:ARG:HH11  | 3:G:88:ARG:HG3   | 1.68                     | 0.58              |
| 6:J:-10:DC:H2''  | 6:J:-9:DA:C8     | 2.38                     | 0.58              |
| 6:J:152:DA:C6    | 6:J:153:DG:C6    | 2.91                     | 0.58              |
| 2:L:51:TYR:O     | 2:L:54:THR:OG1   | 2.19                     | 0.58              |
| 8:V:548:ILE:HD11 | 8:V:560:ALA:HB3  | 1.83                     | 0.58              |
| 1:A:113:HIS:CE1  | 1:E:122:LYS:HE2  | 2.38                     | 0.58              |
| 3:C:70:ALA:HA    | 3:C:82:HIS:NE2   | 2.18                     | 0.58              |
| 4:D:97:LEU:HD12  | 4:D:98:LEU:HG    | 1.86                     | 0.58              |
| 3:G:16:THR:O     | 3:G:19:SER:OG    | 2.16                     | 0.58              |
| 5:I:130:DC:H2''  | 5:I:131:DA:N7    | 2.17                     | 0.58              |
| 1:A:54:TYR:HA    | 1:A:57:SER:OG    | 2.03                     | 0.58              |
| 2:F:93:GLN:O     | 2:F:95:ARG:NH1   | 2.36                     | 0.58              |
| 5:I:214:DC:H2''  | 5:I:215:DT:H72   | 1.85                     | 0.58              |
| 3:Q:112:GLN:HB2  | 3:Q:115:LEU:HG   | 1.85                     | 0.58              |
| 5:I:262:DC:OP1   | 8:V:335:MET:N    | 2.37                     | 0.58              |
| 1:O:100:LEU:HD21 | 2:P:58:LEU:HD13  | 1.84                     | 0.58              |
| 8:V:808:GLN:HG2  | 8:V:885:THR:HA   | 1.85                     | 0.58              |
| 7:U:254:MET:HG3  | 7:U:257:LEU:HD21 | 1.85                     | 0.58              |
| 7:U:581:ASN:ND2  | 7:U:583:GLU:OE2  | 2.35                     | 0.58              |
| 4:D:102:GLU:O    | 4:D:106:HIS:HD2  | 1.85                     | 0.58              |
| 7:U:295:PHE:HB2  | 7:U:376:ASP:HA   | 1.85                     | 0.58              |
| 2:L:60:VAL:O     | 2:L:64:ASN:ND2   | 2.36                     | 0.58              |
| 8:V:966:ARG:O    | 8:V:970:GLU:N    | 2.37                     | 0.58              |
| 1:E:88:ALA:O     | 1:E:92:LEU:HG    | 2.03                     | 0.58              |
| 2:L:75:HIS:NE2   | 4:N:90:GLU:HG3   | 2.19                     | 0.58              |
| 8:V:239:ARG:HH21 | 8:V:270:ASP:HB3  | 1.67                     | 0.58              |
| 7:U:546:ILE:O    | 7:U:605:TYR:OH   | 2.13                     | 0.58              |
| 3:Q:30:VAL:HA    | 3:Q:33:LEU:HB2   | 1.86                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:Q:45:ALA:O     | 3:Q:48:PRO:HD2    | 2.04                     | 0.58              |
| 7:U:311:TYR:CD2  | 7:U:362:PRO:HB3   | 2.39                     | 0.58              |
| 1:K:100:LEU:HD23 | 2:L:58:LEU:HD11   | 1.86                     | 0.58              |
| 1:O:50:GLU:OE1   | 2:P:39:ARG:NE     | 2.21                     | 0.58              |
| 8:V:825:THR:O    | 8:V:829:THR:OG1   | 2.20                     | 0.58              |
| 1:E:83:ARG:HB2   | 2:F:80:THR:HG22   | 1.86                     | 0.57              |
| 2:F:26:ILE:HD11  | 2:F:55:ARG:HB3    | 1.86                     | 0.57              |
| 5:I:132:DG:H1'   | 5:I:133:DA:C8     | 2.39                     | 0.57              |
| 5:I:274:DC:O2    | 6:J:41:DG:N2      | 2.18                     | 0.57              |
| 7:U:372:ASN:HB3  | 7:U:375:MET:HE1   | 1.86                     | 0.57              |
| 7:U:498:LYS:O    | 7:U:501:LEU:HG    | 2.04                     | 0.57              |
| 8:V:422:LEU:HD12 | 8:V:423:PRO:HD2   | 1.84                     | 0.57              |
| 1:E:65:LEU:HB3   | 1:E:69:ARG:NH1    | 2.19                     | 0.57              |
| 7:U:250:CYS:HA   | 7:U:253:LYS:HG2   | 1.86                     | 0.57              |
| 1:K:97:GLU:O     | 1:K:100:LEU:HG    | 2.04                     | 0.57              |
| 2:F:31:LYS:O     | 2:F:35:ARG:HG3    | 2.04                     | 0.57              |
| 5:I:145:DT:H3    | 6:J:171:DG:H1'    | 1.69                     | 0.57              |
| 7:U:201:GLN:NE2  | 7:U:559:ASP:OD2   | 2.36                     | 0.57              |
| 2:L:29:ILE:O     | 2:L:29:ILE:HG13   | 2.04                     | 0.57              |
| 8:V:546:CYS:HB3  | 8:V:560:ALA:HB1   | 1.86                     | 0.57              |
| 8:V:898:VAL:HG23 | 8:V:910:ILE:HB    | 1.85                     | 0.57              |
| 1:A:40:ARG:HG2   | 5:I:84:DC:H5''    | 1.86                     | 0.57              |
| 4:D:87:THR:OG1   | 4:D:90:GLU:OE1    | 2.20                     | 0.57              |
| 2:F:64:ASN:HA    | 2:F:67:ARG:HH22   | 1.70                     | 0.57              |
| 5:I:164:DC:N4    | 6:J:151:DG:H22    | 2.00                     | 0.57              |
| 8:V:1019:ARG:NH1 | 8:V:1023:ARG:HE   | 2.03                     | 0.57              |
| 3:C:100:VAL:HA   | 2:F:96:THR:OG1    | 2.04                     | 0.57              |
| 7:U:313:ARG:HE   | 7:U:619:ARG:HH21  | 1.52                     | 0.57              |
| 3:Q:70:ALA:HA    | 3:Q:82:HIS:CE1    | 2.39                     | 0.57              |
| 5:I:287:DA:H4'   | 5:I:288:DG:H5'    | 1.87                     | 0.57              |
| 5:I:318:DT:H2'   | 5:I:318:DT:OP2    | 2.03                     | 0.57              |
| 7:U:528:GLU:HB3  | 7:U:530:LEU:HD23  | 1.86                     | 0.57              |
| 7:U:646:TYR:O    | 7:U:678:THR:HG21  | 2.04                     | 0.57              |
| 8:V:197:ARG:HG2  | 9:V:1201:ADP:HN61 | 1.70                     | 0.57              |
| 7:U:490:LEU:HG   | 7:U:501:LEU:HD22  | 1.85                     | 0.57              |
| 3:G:29:ARG:HG3   | 3:G:32:ARG:NH2    | 2.20                     | 0.57              |
| 6:J:56:DG:OP2    | 8:V:557:ARG:NH2   | 2.37                     | 0.57              |
| 6:J:151:DG:H1'   | 6:J:152:DA:N7     | 2.20                     | 0.57              |
| 8:V:1016:GLU:OE2 | 8:V:1019:ARG:NH2  | 2.38                     | 0.57              |
| 1:A:125:GLN:O    | 1:A:129:ARG:HG2   | 2.04                     | 0.57              |
| 1:A:131:ARG:CZ   | 1:A:133:GLU:HB3   | 2.35                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:25:PHE:N     | 3:G:56:GLU:OE2   | 2.36                     | 0.57              |
| 7:U:388:ARG:O    | 7:U:391:LEU:HG   | 2.05                     | 0.57              |
| 7:U:455:TYR:HB3  | 7:U:483:LEU:HD13 | 1.87                     | 0.57              |
| 2:L:16:LYS:O     | 2:L:19:ARG:NH2   | 2.35                     | 0.57              |
| 2:L:90:LEU:HA    | 2:L:93:GLN:HE22  | 1.70                     | 0.57              |
| 3:Q:23:LEU:HD12  | 3:Q:24:GLN:H     | 1.69                     | 0.57              |
| 8:V:609:MET:HA   | 8:V:609:MET:HE2  | 1.86                     | 0.57              |
| 5:I:214:DC:H1'   | 5:I:215:DT:C6    | 2.40                     | 0.56              |
| 3:Q:87:VAL:HG22  | 3:Q:93:LEU:HD13  | 1.85                     | 0.56              |
| 8:V:367:LEU:HA   | 8:V:370:LEU:HD12 | 1.87                     | 0.56              |
| 1:E:54:TYR:HB3   | 2:F:40:ARG:CG    | 2.35                     | 0.56              |
| 5:I:289:DG:H21   | 4:N:30:ARG:HH22  | 1.53                     | 0.56              |
| 6:J:-20:DC:H2''  | 6:J:-19:DA:C8    | 2.39                     | 0.56              |
| 7:U:375:MET:HG3  | 7:U:379:GLY:O    | 2.05                     | 0.56              |
| 3:C:39:TYR:HB3   | 4:D:75:SER:HB2   | 1.86                     | 0.56              |
| 3:C:64:GLU:HG3   | 3:C:65:LEU:HD22  | 1.87                     | 0.56              |
| 2:F:26:ILE:HG12  | 2:F:55:ARG:HD3   | 1.86                     | 0.56              |
| 5:I:263:DC:O2    | 6:J:52:DG:N2     | 2.18                     | 0.56              |
| 7:U:206:GLN:HE21 | 7:U:600:GLN:HB2  | 1.69                     | 0.56              |
| 7:U:410:ILE:O    | 7:U:414:THR:HG22 | 2.04                     | 0.56              |
| 7:U:553:ARG:HD3  | 7:U:554:LEU:HD22 | 1.87                     | 0.56              |
| 7:U:647:LYS:HZ1  | 7:U:687:THR:C    | 2.13                     | 0.56              |
| 8:V:896:ILE:CD1  | 8:V:943:TYR:HB3  | 2.35                     | 0.56              |
| 1:A:72:ARG:O     | 1:A:76:GLN:HG3   | 2.05                     | 0.56              |
| 4:D:90:GLU:OE1   | 4:D:90:GLU:N     | 2.21                     | 0.56              |
| 8:V:806:SER:O    | 8:V:808:GLN:NE2  | 2.39                     | 0.56              |
| 8:V:960:GLN:NE2  | 8:V:1054:GLU:OE1 | 2.39                     | 0.56              |
| 3:C:14:ALA:HB1   | 6:J:198:DA:H4'   | 1.88                     | 0.56              |
| 3:C:77:ARG:NH2   | 5:I:132:DG:H5''  | 2.17                     | 0.56              |
| 8:V:120:LYS:H    | 8:V:120:LYS:HD2  | 1.71                     | 0.56              |
| 8:V:277:GLN:HG3  | 8:V:554:HIS:CE1  | 2.40                     | 0.56              |
| 2:B:51:TYR:O     | 2:B:54:THR:OG1   | 2.21                     | 0.56              |
| 6:J:184:DT:H4'   | 6:J:185:DG:OP1   | 2.05                     | 0.56              |
| 3:C:62:ILE:HG13  | 3:C:63:LEU:HD22  | 1.88                     | 0.56              |
| 6:J:27:DC:H2''   | 6:J:28:DT:C5     | 2.41                     | 0.56              |
| 6:J:151:DG:H1'   | 6:J:152:DA:C8    | 2.41                     | 0.56              |
| 7:U:343:ASP:OD2  | 8:V:904:ARG:NH1  | 2.38                     | 0.56              |
| 3:M:97:LEU:HD13  | 3:M:100:VAL:HG21 | 1.88                     | 0.56              |
| 4:R:87:THR:OG1   | 4:R:90:GLU:OE2   | 2.20                     | 0.56              |
| 2:F:90:LEU:HA    | 2:F:93:GLN:HE21  | 1.71                     | 0.56              |
| 7:U:211:GLY:HA3  | 7:U:254:MET:CE   | 2.36                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:U:241:PHE:HD2  | 7:U:242:MET:HE2  | 1.71                     | 0.56              |
| 7:U:364:PRO:O    | 7:U:368:ASN:N    | 2.39                     | 0.56              |
| 2:L:20:LYS:NZ    | 2:L:23:ARG:HD2   | 2.21                     | 0.56              |
| 3:M:55:LEU:O     | 3:M:59:THR:OG1   | 2.14                     | 0.56              |
| 8:V:820:LYS:NZ   | 8:V:866:GLN:HE21 | 2.04                     | 0.56              |
| 5:I:251:DC:H5''  | 1:K:40:ARG:HG2   | 1.87                     | 0.56              |
| 7:U:427:GLN:HB2  | 7:U:536:GLN:NE2  | 2.20                     | 0.56              |
| 7:U:641:LEU:HD23 | 7:U:644:LEU:HD21 | 1.88                     | 0.56              |
| 1:O:90:MET:HE3   | 1:O:90:MET:O     | 2.05                     | 0.56              |
| 8:V:966:ARG:HH22 | 8:V:1064:ASP:HB3 | 1.69                     | 0.56              |
| 1:A:100:LEU:HB3  | 1:A:104:PHE:CZ   | 2.40                     | 0.56              |
| 3:C:76:THR:O     | 4:D:50:GLY:N     | 2.30                     | 0.56              |
| 2:F:71:THR:O     | 2:F:74:GLU:HG3   | 2.05                     | 0.56              |
| 5:I:187:DA:C6    | 5:I:188:DG:C6    | 2.94                     | 0.56              |
| 7:U:637:LEU:HD22 | 7:U:714:TYR:CD2  | 2.41                     | 0.56              |
| 8:V:957:VAL:HG11 | 8:V:1011:ARG:HB3 | 1.88                     | 0.56              |
| 6:J:284:DA:H1'   | 6:J:285:DT:C5'   | 2.35                     | 0.55              |
| 7:U:234:SER:C    | 7:U:235:LEU:HD12 | 2.31                     | 0.55              |
| 7:U:342:VAL:O    | 8:V:928:LYS:HD3  | 2.07                     | 0.55              |
| 2:L:30:THR:HB    | 2:L:32:PRO:HD2   | 1.88                     | 0.55              |
| 1:O:70:LEU:HB2   | 2:P:25:ASN:HB3   | 1.88                     | 0.55              |
| 8:V:983:PRO:HG2  | 8:V:1052:CYS:O   | 2.05                     | 0.55              |
| 8:V:1031:ASP:OD1 | 8:V:1033:TYR:N   | 2.40                     | 0.55              |
| 1:E:98:ALA:O     | 1:E:101:VAL:HG12 | 2.07                     | 0.55              |
| 1:E:131:ARG:HB2  | 1:E:133:GLU:OE1  | 2.06                     | 0.55              |
| 7:U:715:PHE:HA   | 7:U:718:ARG:NH1  | 2.21                     | 0.55              |
| 4:N:65:ASP:OD2   | 4:N:69:ARG:NE    | 2.39                     | 0.55              |
| 8:V:197:ARG:HG2  | 9:V:1201:ADP:N6  | 2.21                     | 0.55              |
| 7:U:267:THR:HB   | 7:U:281:LEU:HD21 | 1.89                     | 0.55              |
| 7:U:383:LEU:H    | 7:U:388:ARG:NH2  | 2.04                     | 0.55              |
| 7:U:431:ARG:NH2  | 7:U:521:PRO:HB3  | 2.22                     | 0.55              |
| 1:O:57:SER:HG    | 2:P:40:ARG:HH21  | 1.48                     | 0.55              |
| 8:V:933:ASN:HB3  | 8:V:936:ARG:HB2  | 1.89                     | 0.55              |
| 5:I:218:DC:N4    | 6:J:97:DG:O6     | 2.34                     | 0.55              |
| 7:U:254:MET:HA   | 7:U:257:LEU:HG   | 1.87                     | 0.55              |
| 1:K:131:ARG:HA   | 1:K:131:ARG:CZ   | 2.36                     | 0.55              |
| 3:M:96:LEU:HD11  | 4:N:100:PRO:HD3  | 1.87                     | 0.55              |
| 1:O:100:LEU:HD11 | 2:P:58:LEU:HD22  | 1.89                     | 0.55              |
| 3:Q:29:ARG:NH1   | 4:R:33:SER:O     | 2.39                     | 0.55              |
| 3:Q:39:TYR:OH    | 4:R:68:GLU:OE1   | 2.25                     | 0.55              |
| 8:V:106:THR:HG22 | 8:V:136:VAL:HB   | 1.88                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:F:31:LYS:HB2   | 2:F:32:PRO:HD3    | 1.88                     | 0.55              |
| 7:U:350:LEU:HB2  | 8:V:902:TYR:O     | 2.06                     | 0.55              |
| 7:U:634:SER:OG   | 7:U:721:GLU:OE1   | 2.17                     | 0.55              |
| 3:G:55:LEU:O     | 3:G:59:THR:HG23   | 2.07                     | 0.55              |
| 5:I:244:DT:H3    | 6:J:71:DA:H61     | 1.53                     | 0.55              |
| 7:U:578:LYS:HG3  | 7:U:583:GLU:OE1   | 2.06                     | 0.55              |
| 8:V:1054:GLU:HG2 | 8:V:1058:ASN:HD21 | 1.71                     | 0.55              |
| 1:A:67:PHE:CE2   | 1:A:93:GLN:HB3    | 2.42                     | 0.55              |
| 5:I:89:DT:H2''   | 5:I:90:DA:C8      | 2.41                     | 0.55              |
| 5:I:269:DG:H2''  | 5:I:270:DA:H8     | 1.72                     | 0.55              |
| 3:M:20:ARG:HD2   | 4:N:118:TYR:CE1   | 2.40                     | 0.55              |
| 3:M:96:LEU:O     | 3:M:99:ARG:NH2    | 2.33                     | 0.55              |
| 3:Q:41:GLU:OE2   | 3:Q:42:ARG:HG3    | 2.07                     | 0.55              |
| 3:C:77:ARG:HA    | 4:D:50:GLY:C      | 2.32                     | 0.55              |
| 1:E:72:ARG:HG2   | 1:E:84:PHE:HE2    | 1.72                     | 0.55              |
| 6:J:132:DC:H2''  | 6:J:133:DA:C8     | 2.42                     | 0.55              |
| 7:U:559:ASP:OD1  | 7:U:560:SER:N     | 2.38                     | 0.55              |
| 1:K:87:SER:HA    | 1:K:90:MET:HE3    | 1.89                     | 0.55              |
| 8:V:797:ARG:HG3  | 8:V:822:ARG:HG2   | 1.87                     | 0.55              |
| 8:V:807:HIS:HE2  | 8:V:937:ILE:HG23  | 1.71                     | 0.55              |
| 8:V:884:PHE:HB3  | 8:V:887:TRP:HD1   | 1.71                     | 0.55              |
| 3:G:43:VAL:HA    | 4:H:86:ILE:HB     | 1.89                     | 0.55              |
| 4:H:34:TYR:OH    | 4:H:64:ASN:OD1    | 2.22                     | 0.55              |
| 7:U:554:LEU:HG   | 7:U:555:HIS:O     | 2.06                     | 0.55              |
| 3:M:51:LEU:HD12  | 3:M:52:ALA:N      | 2.22                     | 0.55              |
| 8:V:111:HIS:HD2  | 8:V:215:ILE:HD13  | 1.71                     | 0.55              |
| 2:B:75:HIS:ND1   | 4:D:93:THR:HG21   | 2.21                     | 0.54              |
| 8:V:122:PHE:CE2  | 8:V:375:PHE:HA    | 2.42                     | 0.54              |
| 6:J:284:DA:C1'   | 6:J:285:DT:C5'    | 2.86                     | 0.54              |
| 7:U:266:PHE:CE2  | 7:U:301:ARG:HB3   | 2.41                     | 0.54              |
| 7:U:635:ALA:O    | 7:U:639:GLU:HG3   | 2.07                     | 0.54              |
| 4:R:76:ARG:HA    | 4:R:79:HIS:HD2    | 1.71                     | 0.54              |
| 4:R:87:THR:H     | 4:R:90:GLU:CD     | 2.15                     | 0.54              |
| 8:V:797:ARG:HG3  | 8:V:798:MET:H     | 1.73                     | 0.54              |
| 1:A:119:ILE:HG12 | 2:B:46:ILE:HA     | 1.88                     | 0.54              |
| 3:G:80:PRO:HA    | 3:G:83:LEU:HD12   | 1.89                     | 0.54              |
| 7:U:480:LEU:O    | 7:U:484:LYS:HG2   | 2.07                     | 0.54              |
| 1:O:59:GLU:CD    | 1:O:60:LEU:H      | 2.15                     | 0.54              |
| 8:V:611:ARG:NE   | 8:V:611:ARG:HA    | 2.22                     | 0.54              |
| 8:V:899:SER:HA   | 8:V:910:ILE:HG21  | 1.89                     | 0.54              |
| 8:V:1071:MET:HG3 | 8:V:1072:LYS:HG2  | 1.89                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:115:LEU:HD13  | 2:F:44:LYS:HB2   | 1.90                     | 0.54              |
| 5:I:327:DT:H2'    | 5:I:327:DT:OP2   | 2.06                     | 0.54              |
| 6:J:102:DA:H2''   | 6:J:103:DG:H8    | 1.73                     | 0.54              |
| 7:U:313:ARG:NE    | 7:U:619:ARG:HH21 | 2.05                     | 0.54              |
| 7:U:464:PHE:HZ    | 7:U:476:LEU:HD22 | 1.73                     | 0.54              |
| 3:Q:18:SER:OG     | 3:Q:25:PHE:O     | 2.25                     | 0.54              |
| 5:I:181:DG:H2'    | 5:I:182:DT:H71   | 1.90                     | 0.54              |
| 6:J:1:DT:H2''     | 6:J:2:DC:C6      | 2.43                     | 0.54              |
| 7:U:204:SER:N     | 7:U:207:ASP:OD2  | 2.40                     | 0.54              |
| 8:V:117:GLY:HA2   | 8:V:120:LYS:HD3  | 1.89                     | 0.54              |
| 1:O:61:LEU:HD13   | 2:P:36:ARG:HB3   | 1.90                     | 0.54              |
| 5:I:153:DG:H1'    | 5:I:154:DT:H5'   | 1.90                     | 0.54              |
| 4:N:106:HIS:O     | 4:N:110:GLU:HG3  | 2.07                     | 0.54              |
| 8:V:305:ILE:O     | 8:V:309:GLU:HG2  | 2.07                     | 0.54              |
| 8:V:887:TRP:HA    | 8:V:891:GLU:HB2  | 1.90                     | 0.54              |
| 1:E:69:ARG:HB3    | 2:F:25:ASN:OD1   | 2.08                     | 0.54              |
| 1:E:128:ARG:NH2   | 1:E:133:GLU:HB3  | 2.22                     | 0.54              |
| 2:F:91:LYS:HZ1    | 4:H:76:ARG:HH12  | 1.55                     | 0.54              |
| 1:K:85:GLN:O      | 1:K:89:VAL:HG23  | 2.07                     | 0.54              |
| 2:L:58:LEU:O      | 2:L:61:PHE:HB3   | 2.07                     | 0.54              |
| 7:U:328:PRO:O     | 7:U:358:ASN:ND2  | 2.37                     | 0.54              |
| 8:V:248:PHE:N     | 8:V:297:ASP:O    | 2.40                     | 0.54              |
| 8:V:824:TRP:HA    | 8:V:827:LYS:HG2  | 1.89                     | 0.54              |
| 1:E:54:TYR:HA     | 1:E:57:SER:OG    | 2.08                     | 0.54              |
| 3:G:79:ILE:HG12   | 3:G:82:HIS:ND1   | 2.23                     | 0.54              |
| 5:I:174:DA:H2''   | 5:I:175:DA:C8    | 2.41                     | 0.54              |
| 6:J:123:DC:H4'    | 4:R:30:ARG:HD2   | 1.89                     | 0.54              |
| 7:U:447:LEU:O     | 7:U:451:ILE:HG12 | 2.08                     | 0.54              |
| 1:K:123:ASP:OD1   | 1:O:113:HIS:NE2  | 2.39                     | 0.54              |
| 3:M:95:LYS:NZ     | 4:N:100:PRO:HG3  | 2.22                     | 0.54              |
| 1:O:52:ARG:NH1    | 1:O:52:ARG:HB2   | 2.23                     | 0.54              |
| 8:V:1022:ILE:HG21 | 8:V:1034:PHE:HB3 | 1.89                     | 0.54              |
| 3:G:78:ILE:O      | 4:H:52:SER:N     | 2.38                     | 0.53              |
| 5:I:147:DA:H5'    | 6:J:171:DG:H5''  | 1.90                     | 0.53              |
| 5:I:235:DT:H2''   | 5:I:236:DA:C8    | 2.42                     | 0.53              |
| 5:I:332:DG:N2     | 6:J:-16:DT:O2    | 2.41                     | 0.53              |
| 1:K:119:ILE:O     | 1:K:120:MET:HE2  | 2.07                     | 0.53              |
| 4:D:62:PHE:HD1    | 2:F:98:TYR:HE2   | 1.56                     | 0.53              |
| 4:H:96:ARG:HG2    | 4:H:96:ARG:HH11  | 1.73                     | 0.53              |
| 7:U:606:HIS:CD2   | 7:U:627:TRP:HD1  | 2.27                     | 0.53              |
| 2:P:47:SER:HB3    | 2:P:50:ILE:HG12  | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:Q:52:ALA:O     | 3:Q:55:LEU:HB2   | 2.08                     | 0.53              |
| 4:R:90:GLU:CD    | 4:R:90:GLU:H     | 2.11                     | 0.53              |
| 8:V:228:THR:OG1  | 9:V:1201:ADP:O3B | 2.22                     | 0.53              |
| 2:B:31:LYS:HG3   | 2:B:51:TYR:CE1   | 2.43                     | 0.53              |
| 3:G:31:HIS:CD2   | 3:G:35:ARG:HH11  | 2.25                     | 0.53              |
| 6:J:150:DC:H2"   | 6:J:151:DG:C8    | 2.43                     | 0.53              |
| 7:U:483:LEU:HA   | 7:U:486:ILE:HG12 | 1.90                     | 0.53              |
| 7:U:483:LEU:HD21 | 7:U:512:LEU:HD13 | 1.90                     | 0.53              |
| 8:V:201:ILE:HG22 | 8:V:205:ASN:OD1  | 2.09                     | 0.53              |
| 3:C:29:ARG:HG3   | 3:C:32:ARG:NH2   | 2.22                     | 0.53              |
| 6:J:72:DC:H2"    | 6:J:73:DA:C8     | 2.44                     | 0.53              |
| 8:V:614:ARG:NH2  | 9:V:1201:ADP:O2B | 2.36                     | 0.53              |
| 4:D:87:THR:H     | 4:D:90:GLU:CD    | 2.16                     | 0.53              |
| 8:V:436:MET:HG2  | 8:V:500:ASN:ND2  | 2.24                     | 0.53              |
| 8:V:826:ALA:HA   | 8:V:831:TYR:HB2  | 1.91                     | 0.53              |
| 4:N:72:GLY:O     | 4:N:76:ARG:HG3   | 2.09                     | 0.53              |
| 7:U:263:ASP:HB3  | 7:U:281:LEU:HD23 | 1.90                     | 0.53              |
| 7:U:556:SER:HB3  | 7:U:566:PHE:CD2  | 2.43                     | 0.53              |
| 1:K:62:ILE:HB    | 1:K:93:GLN:NE2   | 2.24                     | 0.53              |
| 1:K:108:ASN:HA   | 1:K:119:ILE:HD11 | 1.90                     | 0.53              |
| 2:P:75:HIS:NE2   | 4:R:89:ARG:HG2   | 2.24                     | 0.53              |
| 7:U:162:TYR:HA   | 7:U:613:HIS:HE1  | 1.73                     | 0.53              |
| 7:U:316:ARG:HB2  | 7:U:318:GLN:OE1  | 2.07                     | 0.53              |
| 2:P:93:GLN:OE1   | 2:P:95:ARG:HG3   | 2.08                     | 0.53              |
| 8:V:989:LYS:O    | 8:V:991:THR:HG23 | 2.09                     | 0.53              |
| 8:V:1057:PHE:O   | 8:V:1061:ILE:N   | 2.34                     | 0.53              |
| 3:G:81:ARG:HH12  | 3:G:107:VAL:N    | 2.06                     | 0.53              |
| 8:V:958:LYS:O    | 8:V:961:GLN:HB3  | 2.09                     | 0.53              |
| 3:C:17:ARG:HA    | 3:C:20:ARG:HD2   | 1.89                     | 0.53              |
| 4:D:37:TYR:O     | 4:D:41:VAL:HG22  | 2.09                     | 0.53              |
| 4:D:95:VAL:HG13  | 4:D:99:LEU:HD12  | 1.91                     | 0.53              |
| 2:F:77:LYS:HZ3   | 4:H:89:ARG:NH2   | 2.07                     | 0.53              |
| 5:I:164:DC:H2"   | 5:I:165:DG:C8    | 2.44                     | 0.53              |
| 7:U:197:HIS:H    | 7:U:200:LEU:HD12 | 1.73                     | 0.53              |
| 7:U:303:ARG:HB2  | 7:U:371:TYR:OH   | 2.09                     | 0.53              |
| 1:K:113:HIS:CG   | 1:O:126:LEU:HG   | 2.44                     | 0.53              |
| 8:V:439:LYS:O    | 8:V:443:LYS:HG3  | 2.09                     | 0.53              |
| 8:V:957:VAL:HA   | 8:V:960:GLN:HB2  | 1.90                     | 0.53              |
| 2:F:50:ILE:O     | 2:F:54:THR:HG23  | 2.10                     | 0.52              |
| 7:U:161:GLN:H    | 7:U:161:GLN:CD   | 2.17                     | 0.52              |
| 7:U:227:VAL:HB   | 7:U:232:ASP:HB3  | 1.90                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:U:506:TYR:OH   | 7:U:522:LEU:O    | 2.26                     | 0.52              |
| 7:U:706:LEU:HD13 | 7:U:709:PHE:CD2  | 2.44                     | 0.52              |
| 8:V:947:ILE:O    | 8:V:951:GLU:HG3  | 2.09                     | 0.52              |
| 8:V:1038:THR:OG1 | 8:V:1041:GLU:OE1 | 2.16                     | 0.52              |
| 1:A:47:ALA:O     | 1:A:51:ILE:HG13  | 2.09                     | 0.52              |
| 1:A:59:GLU:OE1   | 1:A:59:GLU:N     | 2.42                     | 0.52              |
| 4:D:37:TYR:HA    | 4:D:40:LYS:NZ    | 2.25                     | 0.52              |
| 2:F:33:ALA:O     | 2:F:37:LEU:HG    | 2.09                     | 0.52              |
| 2:L:15:ALA:HA    | 2:L:17:ARG:HH12  | 1.73                     | 0.52              |
| 1:O:96:SER:O     | 1:O:99:TYR:HB3   | 2.09                     | 0.52              |
| 8:V:279:ASP:N    | 8:V:282:GLU:HB2  | 2.24                     | 0.52              |
| 1:A:131:ARG:NH2  | 1:A:133:GLU:HB3  | 2.24                     | 0.52              |
| 7:U:179:ALA:O    | 7:U:182:ILE:N    | 2.42                     | 0.52              |
| 3:M:78:ILE:HA    | 3:M:82:HIS:ND1   | 2.24                     | 0.52              |
| 3:M:79:ILE:HG13  | 3:M:82:HIS:H     | 1.75                     | 0.52              |
| 2:F:90:LEU:HA    | 2:F:93:GLN:HG2   | 1.91                     | 0.52              |
| 5:I:233:DC:H2''  | 5:I:234:DG:C8    | 2.44                     | 0.52              |
| 6:J:0:DC:OP2     | 6:J:0:DC:H2'     | 2.09                     | 0.52              |
| 7:U:538:PHE:O    | 7:U:551:MET:N    | 2.31                     | 0.52              |
| 2:L:83:ALA:O     | 2:L:87:VAL:HG23  | 2.09                     | 0.52              |
| 2:P:34:ILE:HG21  | 2:P:51:TYR:HD1   | 1.74                     | 0.52              |
| 8:V:413:ILE:HD11 | 8:V:655:ARG:CZ   | 2.38                     | 0.52              |
| 8:V:980:LEU:HG   | 8:V:1056:GLU:OE1 | 2.09                     | 0.52              |
| 8:V:1004:LEU:O   | 8:V:1007:TYR:HB2 | 2.10                     | 0.52              |
| 5:I:258:DA:H4'   | 1:K:63:ARG:NH1   | 2.25                     | 0.52              |
| 7:U:654:GLU:HA   | 7:U:692:LYS:HB2  | 1.92                     | 0.52              |
| 3:Q:92:GLU:HG2   | 4:R:103:LEU:HG   | 1.91                     | 0.52              |
| 8:V:409:LEU:HD23 | 8:V:411:ARG:HH11 | 1.74                     | 0.52              |
| 8:V:922:GLU:OE2  | 8:V:926:TYR:HB2  | 2.10                     | 0.52              |
| 4:D:58:ILE:HG23  | 2:F:98:TYR:HB3   | 1.92                     | 0.52              |
| 6:J:143:DT:H2''  | 6:J:144:DC:C6    | 2.44                     | 0.52              |
| 3:Q:29:ARG:NE    | 4:R:32:GLU:OE2   | 2.43                     | 0.52              |
| 4:R:77:LEU:HD23  | 4:R:80:TYR:CD2   | 2.45                     | 0.52              |
| 1:A:60:LEU:HD22  | 1:A:64:LYS:NZ    | 2.24                     | 0.52              |
| 1:A:76:GLN:HB3   | 7:U:244:ILE:HD11 | 1.91                     | 0.52              |
| 7:U:651:PRO:HG3  | 7:U:700:ARG:NH2  | 2.25                     | 0.52              |
| 3:M:18:SER:OG    | 3:M:25:PHE:O     | 2.26                     | 0.52              |
| 3:Q:31:HIS:O     | 3:Q:35:ARG:HB2   | 2.09                     | 0.52              |
| 8:V:223:MET:SD   | 8:V:610:ASP:HB2  | 2.49                     | 0.52              |
| 2:B:71:THR:HA    | 2:B:74:GLU:OE2   | 2.09                     | 0.52              |
| 1:E:84:PHE:HA    | 2:F:81:VAL:HG22  | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:I:131:DA:H4'   | 5:I:132:DG:OP1   | 2.09                     | 0.52              |
| 7:U:154:LEU:HD13 | 7:U:427:GLN:HG2  | 1.91                     | 0.52              |
| 7:U:539:PHE:HA   | 7:U:550:TYR:CD1  | 2.43                     | 0.52              |
| 4:R:115:VAL:O    | 4:R:119:THR:HG23 | 2.09                     | 0.52              |
| 8:V:824:TRP:HE1  | 8:V:828:LYS:HD2  | 1.73                     | 0.52              |
| 8:V:838:VAL:HG22 | 8:V:857:LEU:HD23 | 1.91                     | 0.52              |
| 8:V:1054:GLU:O   | 8:V:1058:ASN:ND2 | 2.42                     | 0.52              |
| 3:G:28:GLY:HA3   | 5:I:30:DA:H3'    | 1.92                     | 0.52              |
| 7:U:171:PRO:HD3  | 7:U:685:ILE:HG13 | 1.92                     | 0.52              |
| 7:U:375:MET:SD   | 7:U:382:ALA:HB3  | 2.50                     | 0.52              |
| 4:N:101:GLY:O    | 4:N:105:LYS:HG3  | 2.10                     | 0.52              |
| 2:P:75:HIS:HE1   | 4:R:90:GLU:HA    | 1.75                     | 0.52              |
| 7:U:215:TYR:HB2  | 7:U:223:ALA:O    | 2.09                     | 0.52              |
| 7:U:633:ASP:OD1  | 7:U:635:ALA:N    | 2.42                     | 0.52              |
| 1:K:60:LEU:HB2   | 1:K:93:GLN:NE2   | 2.25                     | 0.52              |
| 1:K:97:GLU:HA    | 1:K:100:LEU:HG   | 1.92                     | 0.52              |
| 1:K:131:ARG:NH2  | 1:O:131:ARG:HA   | 2.25                     | 0.52              |
| 2:L:44:LYS:HG2   | 3:Q:115:LEU:HD22 | 1.92                     | 0.52              |
| 3:M:57:TYR:O     | 3:M:61:GLU:HB2   | 2.10                     | 0.52              |
| 8:V:965:ARG:HA   | 8:V:1005:PHE:CZ  | 2.44                     | 0.52              |
| 8:V:992:TYR:HB2  | 8:V:1045:ARG:CZ  | 2.40                     | 0.52              |
| 4:D:37:TYR:HA    | 4:D:40:LYS:HZ2   | 1.75                     | 0.51              |
| 1:E:100:LEU:O    | 1:E:103:LEU:HB2  | 2.10                     | 0.51              |
| 7:U:327:LYS:NZ   | 8:V:1006:LYS:HD3 | 2.25                     | 0.51              |
| 2:L:16:LYS:HE3   | 2:L:19:ARG:HD3   | 1.90                     | 0.51              |
| 3:M:54:VAL:HG12  | 3:M:58:LEU:HD23  | 1.92                     | 0.51              |
| 4:R:90:GLU:OE2   | 4:R:90:GLU:N     | 2.20                     | 0.51              |
| 8:V:111:HIS:CD2  | 8:V:215:ILE:HD13 | 2.45                     | 0.51              |
| 8:V:769:ARG:NH1  | 8:V:771:ARG:HH11 | 2.09                     | 0.51              |
| 2:B:59:LYS:O     | 2:B:63:GLU:HG3   | 2.10                     | 0.51              |
| 3:C:26:PRO:HD3   | 4:D:37:TYR:CZ    | 2.46                     | 0.51              |
| 3:G:26:PRO:HG3   | 4:H:37:TYR:CE1   | 2.46                     | 0.51              |
| 7:U:452:GLN:HG3  | 7:U:509:TRP:HH2  | 1.75                     | 0.51              |
| 8:V:556:ASP:OD1  | 8:V:559:GLN:NE2  | 2.42                     | 0.51              |
| 8:V:968:LEU:HD13 | 8:V:1005:PHE:CD1 | 2.43                     | 0.51              |
| 1:E:72:ARG:HG2   | 1:E:84:PHE:CE2   | 2.46                     | 0.51              |
| 1:E:93:GLN:O     | 1:E:97:GLU:OE1   | 2.29                     | 0.51              |
| 4:N:60:ASN:O     | 4:N:64:ASN:ND2   | 2.44                     | 0.51              |
| 8:V:955:LYS:HA   | 8:V:958:LYS:HD2  | 1.92                     | 0.51              |
| 4:H:54:LYS:O     | 4:H:58:ILE:HG12  | 2.10                     | 0.51              |
| 6:J:56:DG:H8     | 8:V:551:SER:HB3  | 1.75                     | 0.51              |

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| Atom-1          | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 7:U:184:LYS:CE  | 8:V:1030:LEU:HA   | 2.41                     | 0.51              |
| 7:U:411:TYR:CE1 | 8:V:1033:TYR:HD1  | 2.28                     | 0.51              |
| 8:V:982:HIS:O   | 8:V:984:PRO:HD3   | 2.11                     | 0.51              |
| 1:E:103:LEU:O   | 1:E:107:THR:HG23  | 2.10                     | 0.51              |
| 7:U:228:LYS:N   | 7:U:232:ASP:OD2   | 2.43                     | 0.51              |
| 7:U:594:GLY:HA2 | 7:U:597:MET:HB2   | 1.93                     | 0.51              |
| 1:K:71:VAL:HG21 | 1:K:92:LEU:HD13   | 1.93                     | 0.51              |
| 8:V:189:PRO:HB2 | 8:V:191:TYR:CE1   | 2.46                     | 0.51              |
| 8:V:480:TYR:CD1 | 8:V:486:GLU:HB2   | 2.45                     | 0.51              |
| 8:V:933:ASN:HB3 | 8:V:936:ARG:HE    | 1.75                     | 0.51              |
| 1:A:118:THR:OG1 | 2:B:45:ARG:HD3    | 2.10                     | 0.51              |
| 3:G:16:THR:O    | 3:G:20:ARG:HG3    | 2.11                     | 0.51              |
| 5:I:328:DC:H2'' | 5:I:329:DA:C8     | 2.46                     | 0.51              |
| 7:U:215:TYR:HB3 | 7:U:226:ILE:HG23  | 1.91                     | 0.51              |
| 3:C:79:ILE:HG12 | 3:C:82:HIS:ND1    | 2.26                     | 0.51              |
| 5:I:161:DG:N2   | 6:J:155:DT:O4'    | 2.44                     | 0.51              |
| 5:I:215:DT:C4   | 5:I:216:DA:C6     | 2.99                     | 0.51              |
| 5:I:317:DG:C2   | 6:J:-1:DG:C2      | 2.98                     | 0.51              |
| 7:U:197:HIS:O   | 7:U:201:GLN:HG3   | 2.11                     | 0.51              |
| 7:U:461:LYS:HD3 | 7:U:464:PHE:HB2   | 1.92                     | 0.51              |
| 2:L:83:ALA:HA   | 2:L:86:VAL:HG12   | 1.93                     | 0.51              |
| 2:L:90:LEU:HD13 | 2:L:93:GLN:NE2    | 2.25                     | 0.51              |
| 8:V:809:LEU:HB2 | 8:V:884:PHE:HD1   | 1.76                     | 0.51              |
| 1:A:48:LEU:HB3  | 1:A:52:ARG:NH1    | 2.25                     | 0.51              |
| 1:E:126:LEU:O   | 1:E:130:ILE:HG12  | 2.11                     | 0.51              |
| 2:F:58:LEU:O    | 2:F:62:LEU:HG     | 2.11                     | 0.51              |
| 5:I:89:DT:H2''  | 5:I:90:DA:N7      | 2.26                     | 0.51              |
| 5:I:261:DG:C2   | 5:I:262:DC:C2     | 2.99                     | 0.51              |
| 3:Q:64:GLU:OE2  | 3:Q:65:LEU:HG     | 2.10                     | 0.51              |
| 2:F:92:ARG:HD2  | 2:F:92:ARG:C      | 2.36                     | 0.51              |
| 4:N:115:VAL:O   | 4:N:119:THR:N     | 2.28                     | 0.51              |
| 8:V:305:ILE:O   | 8:V:309:GLU:N     | 2.44                     | 0.51              |
| 8:V:827:LYS:HD2 | 8:V:864:ASN:CB    | 2.37                     | 0.51              |
| 8:V:894:LYS:O   | 8:V:898:VAL:HG13  | 2.10                     | 0.51              |
| 7:U:578:LYS:HG2 | 7:U:584:TYR:CE2   | 2.46                     | 0.51              |
| 7:U:619:ARG:O   | 7:U:619:ARG:HD3   | 2.11                     | 0.51              |
| 7:U:732:PRO:O   | 7:U:735:ARG:HG2   | 2.10                     | 0.51              |
| 8:V:614:ARG:NH2 | 10:V:1202:BEF:F3  | 2.32                     | 0.51              |
| 8:V:1057:PHE:O  | 8:V:1061:ILE:HG13 | 2.11                     | 0.51              |
| 7:U:148:THR:N   | 7:U:431:ARG:HH22  | 2.08                     | 0.50              |
| 4:R:76:ARG:HA   | 4:R:79:HIS:CD2    | 2.46                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:V:272:ASN:HB3  | 8:V:296:PHE:HA   | 1.93                     | 0.50              |
| 8:V:975:PHE:C    | 8:V:998:ARG:HH21 | 2.16                     | 0.50              |
| 1:A:90:MET:O     | 1:A:94:GLU:OE1   | 2.29                     | 0.50              |
| 5:I:72:DC:H2''   | 5:I:73:DG:C8     | 2.46                     | 0.50              |
| 5:I:101:DG:H1'   | 5:I:102:DG:C8    | 2.46                     | 0.50              |
| 7:U:149:SER:OG   | 7:U:150:VAL:N    | 2.42                     | 0.50              |
| 7:U:679:THR:O    | 7:U:682:ASN:ND2  | 2.44                     | 0.50              |
| 3:Q:17:ARG:NH2   | 3:Q:28:GLY:HA2   | 2.26                     | 0.50              |
| 8:V:508:ASP:OD1  | 8:V:541:ARG:NH1  | 2.43                     | 0.50              |
| 8:V:900:GLY:HA3  | 8:V:947:ILE:HA   | 1.93                     | 0.50              |
| 8:V:942:LYS:HA   | 8:V:945:LYS:HD2  | 1.92                     | 0.50              |
| 4:H:73:GLU:O     | 4:H:77:LEU:HG    | 2.10                     | 0.50              |
| 6:J:-13:DG:H2''  | 6:J:-12:DA:C8    | 2.46                     | 0.50              |
| 7:U:255:ASN:OD1  | 7:U:380:ILE:HG22 | 2.12                     | 0.50              |
| 7:U:303:ARG:NH2  | 7:U:371:TYR:HA   | 2.27                     | 0.50              |
| 7:U:407:HIS:O    | 7:U:411:TYR:HD2  | 1.94                     | 0.50              |
| 7:U:451:ILE:HD12 | 7:U:455:TYR:OH   | 2.11                     | 0.50              |
| 3:M:95:LYS:HE3   | 4:N:100:PRO:HG3  | 1.93                     | 0.50              |
| 4:N:102:GLU:HG3  | 4:N:106:HIS:HE1  | 1.77                     | 0.50              |
| 8:V:887:TRP:HE3  | 8:V:891:GLU:HB3  | 1.77                     | 0.50              |
| 8:V:896:ILE:HD12 | 8:V:930:PHE:CZ   | 2.45                     | 0.50              |
| 1:A:93:GLN:O     | 1:A:97:GLU:OE1   | 2.29                     | 0.50              |
| 4:H:109:SER:HB3  | 4:H:113:LYS:HZ1  | 1.76                     | 0.50              |
| 6:J:40:DA:H2''   | 6:J:41:DG:H8     | 1.75                     | 0.50              |
| 7:U:189:ILE:HA   | 7:U:196:PHE:CE2  | 2.47                     | 0.50              |
| 3:M:79:ILE:HG12  | 3:M:82:HIS:CE1   | 2.46                     | 0.50              |
| 1:O:67:PHE:CE2   | 1:O:93:GLN:HB2   | 2.46                     | 0.50              |
| 3:Q:51:LEU:HD12  | 3:Q:52:ALA:N     | 2.26                     | 0.50              |
| 4:R:64:ASN:O     | 4:R:67:PHE:HB3   | 2.11                     | 0.50              |
| 8:V:205:ASN:HA   | 8:V:208:VAL:HG22 | 1.93                     | 0.50              |
| 8:V:532:ASP:OD1  | 8:V:547:ARG:NH1  | 2.43                     | 0.50              |
| 6:J:184:DT:H2''  | 6:J:185:DG:C5    | 2.47                     | 0.50              |
| 7:U:182:ILE:O    | 7:U:185:LEU:HB2  | 2.12                     | 0.50              |
| 7:U:325:ILE:H    | 7:U:325:ILE:HD12 | 1.76                     | 0.50              |
| 7:U:343:ASP:HB2  | 8:V:931:TRP:CZ3  | 2.46                     | 0.50              |
| 1:K:88:ALA:O     | 1:K:92:LEU:HG    | 2.12                     | 0.50              |
| 1:K:111:ALA:HB1  | 1:K:116:ARG:HB2  | 1.93                     | 0.50              |
| 4:N:73:GLU:O     | 4:N:77:LEU:N     | 2.34                     | 0.50              |
| 1:O:104:PHE:HE2  | 2:P:37:LEU:HB3   | 1.76                     | 0.50              |
| 2:P:72:TYR:OH    | 2:P:92:ARG:HG3   | 2.11                     | 0.50              |
| 4:D:88:SER:HA    | 4:D:91:ILE:HG22  | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:I:310:DC:H2''  | 5:I:311:DC:C6    | 2.47                     | 0.50              |
| 7:U:724:LYS:O    | 7:U:728:ALA:N    | 2.45                     | 0.50              |
| 8:V:998:ARG:O    | 8:V:1002:LEU:HG  | 2.11                     | 0.50              |
| 4:D:91:ILE:O     | 4:D:95:VAL:HG23  | 2.12                     | 0.50              |
| 1:E:62:ILE:HB    | 1:E:93:GLN:NE2   | 2.24                     | 0.50              |
| 5:I:160:DA:H3'   | 5:I:161:DG:H8    | 1.75                     | 0.50              |
| 6:J:116:DA:C6    | 6:J:117:DA:C6    | 3.00                     | 0.50              |
| 6:J:119:DT:H2''  | 6:J:120:DG:C8    | 2.46                     | 0.50              |
| 7:U:453:SER:O    | 7:U:457:ILE:HG12 | 2.12                     | 0.50              |
| 7:U:494:VAL:HG23 | 7:U:497:GLU:H    | 1.77                     | 0.50              |
| 8:V:1054:GLU:O   | 8:V:1058:ASN:N   | 2.44                     | 0.50              |
| 4:D:92:GLN:HE22  | 4:D:96:ARG:NH1   | 2.10                     | 0.50              |
| 5:I:261:DG:C8    | 5:I:261:DG:H5'   | 2.46                     | 0.50              |
| 2:L:30:THR:O     | 2:L:34:ILE:HG13  | 2.11                     | 0.50              |
| 2:L:84:MET:SD    | 2:L:85:ASP:N     | 2.85                     | 0.50              |
| 8:V:248:PHE:HB2  | 8:V:298:VAL:HG22 | 1.94                     | 0.50              |
| 2:F:32:PRO:O     | 2:F:36:ARG:HG3   | 2.12                     | 0.50              |
| 2:F:56:GLY:O     | 2:F:60:VAL:HG23  | 2.12                     | 0.50              |
| 5:I:303:DT:H2''  | 5:I:304:DA:H8    | 1.76                     | 0.50              |
| 6:J:56:DG:C8     | 8:V:551:SER:HB3  | 2.47                     | 0.50              |
| 1:K:97:GLU:O     | 1:K:101:VAL:HG23 | 2.12                     | 0.50              |
| 2:L:66:ILE:O     | 2:L:70:VAL:HG22  | 2.12                     | 0.50              |
| 3:Q:67:GLY:HA3   | 4:R:46:HIS:CD2   | 2.47                     | 0.50              |
| 8:V:284:ALA:O    | 8:V:287:ILE:N    | 2.45                     | 0.50              |
| 8:V:327:HIS:O    | 8:V:330:LYS:NZ   | 2.35                     | 0.50              |
| 8:V:797:ARG:CG   | 8:V:822:ARG:HG2  | 2.42                     | 0.50              |
| 4:D:73:GLU:O     | 4:D:77:LEU:HG    | 2.11                     | 0.49              |
| 6:J:131:DG:C2    | 6:J:132:DC:C2    | 3.00                     | 0.49              |
| 6:J:149:DT:H2''  | 6:J:150:DC:C5    | 2.47                     | 0.49              |
| 7:U:402:HIS:O    | 7:U:404:SER:N    | 2.45                     | 0.49              |
| 7:U:403:SER:HB2  | 7:U:406:ILE:HG12 | 1.94                     | 0.49              |
| 7:U:482:ILE:HA   | 7:U:485:GLU:HG2  | 1.93                     | 0.49              |
| 8:V:261:LEU:HD22 | 8:V:275:ILE:HG13 | 1.93                     | 0.49              |
| 8:V:908:GLN:OE1  | 8:V:912:ARG:NH1  | 2.44                     | 0.49              |
| 1:A:52:ARG:C     | 1:A:56:LYS:HZ2   | 2.20                     | 0.49              |
| 1:A:96:SER:O     | 1:A:100:LEU:HD23 | 2.12                     | 0.49              |
| 1:A:109:LEU:HB3  | 1:E:126:LEU:HD11 | 1.94                     | 0.49              |
| 1:A:124:ILE:O    | 1:A:128:ARG:HG3  | 2.13                     | 0.49              |
| 3:C:81:ARG:NH1   | 3:C:105:GLY:O    | 2.44                     | 0.49              |
| 1:E:59:GLU:N     | 2:F:40:ARG:HH22  | 2.11                     | 0.49              |
| 7:U:313:ARG:HA   | 7:U:316:ARG:HD2  | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:U:342:VAL:HG22  | 8:V:928:LYS:HD3   | 1.93                     | 0.49              |
| 1:K:131:ARG:CZ    | 1:O:131:ARG:HA    | 2.41                     | 0.49              |
| 8:V:961:GLN:OE1   | 8:V:1009:LEU:HB2  | 2.12                     | 0.49              |
| 1:A:48:LEU:HD23   | 1:A:52:ARG:NH2    | 2.27                     | 0.49              |
| 1:E:53:ARG:NH2    | 1:E:54:TYR:OH     | 2.45                     | 0.49              |
| 3:G:77:ARG:HA     | 4:H:50:GLY:C      | 2.37                     | 0.49              |
| 7:U:310:GLY:O     | 7:U:311:TYR:HD1   | 1.94                     | 0.49              |
| 7:U:329:LYS:HB3   | 7:U:356:THR:O     | 2.11                     | 0.49              |
| 3:M:67:GLY:O      | 3:M:71:ARG:HG2    | 2.12                     | 0.49              |
| 3:Q:102:ILE:HG23  | 3:Q:105:GLY:HA3   | 1.93                     | 0.49              |
| 8:V:362:GLU:O     | 8:V:366:LEU:HD12  | 2.13                     | 0.49              |
| 8:V:807:HIS:HE1   | 8:V:937:ILE:HG12  | 1.77                     | 0.49              |
| 8:V:906:SER:HB3   | 8:V:909:ALA:HB3   | 1.94                     | 0.49              |
| 3:C:101:THR:O     | 2:F:97:LEU:HD12   | 2.11                     | 0.49              |
| 2:F:87:VAL:O      | 2:F:90:LEU:HG     | 2.12                     | 0.49              |
| 7:U:338:GLN:HE22  | 8:V:909:ALA:H     | 1.61                     | 0.49              |
| 2:L:77:LYS:C      | 2:L:78:ARG:HD2    | 2.38                     | 0.49              |
| 4:N:43:LYS:HA     | 4:N:47:PRO:HA     | 1.94                     | 0.49              |
| 8:V:320:TYR:HA    | 8:V:347:ASN:O     | 2.12                     | 0.49              |
| 2:B:35:ARG:O      | 2:B:39:ARG:HG2    | 2.13                     | 0.49              |
| 4:D:43:LYS:HE3    | 4:D:47:PRO:O      | 2.12                     | 0.49              |
| 2:F:64:ASN:HA     | 2:F:67:ARG:HH12   | 1.77                     | 0.49              |
| 5:I:258:DA:H2'    | 1:K:65:LEU:HD12   | 1.94                     | 0.49              |
| 6:J:104:DC:H2'    | 6:J:105:DT:C6     | 2.48                     | 0.49              |
| 1:K:62:ILE:HB     | 1:K:93:GLN:HE21   | 1.77                     | 0.49              |
| 4:R:113:LYS:HD2   | 4:R:114:ALA:N     | 2.27                     | 0.49              |
| 1:A:126:LEU:O     | 1:A:130:ILE:HG12  | 2.13                     | 0.49              |
| 4:D:73:GLU:OE1    | 4:D:73:GLU:HA     | 2.13                     | 0.49              |
| 4:D:106:HIS:HE2   | 7:U:735:ARG:HG3   | 1.77                     | 0.49              |
| 6:J:61:DA:H2''    | 6:J:62:DA:H8      | 1.77                     | 0.49              |
| 7:U:444:PHE:CE2   | 7:U:502:LEU:HD11  | 2.48                     | 0.49              |
| 4:R:36:ILE:O      | 4:R:40:LYS:HG3    | 2.13                     | 0.49              |
| 8:V:799:PRO:HG3   | 8:V:822:ARG:NE    | 2.28                     | 0.49              |
| 1:A:57:SER:HB2    | 1:A:59:GLU:OE1    | 2.12                     | 0.49              |
| 3:C:94:ASN:O      | 3:C:98:GLY:N      | 2.46                     | 0.49              |
| 4:H:107:ALA:HA    | 4:H:110:GLU:OE2   | 2.13                     | 0.49              |
| 5:I:317:DG:C2     | 6:J:-1:DG:N2      | 2.80                     | 0.49              |
| 8:V:1027:LEU:HD12 | 8:V:1030:LEU:HD12 | 1.94                     | 0.49              |
| 4:D:89:ARG:O      | 4:D:93:THR:HG23   | 2.12                     | 0.49              |
| 2:F:93:GLN:HG3    | 2:F:95:ARG:HG2    | 1.95                     | 0.49              |
| 1:K:61:LEU:HD12   | 2:L:36:ARG:HB3    | 1.94                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:116:ARG:HH22 | 1:K:123:ASP:CG    | 2.20                     | 0.49              |
| 3:M:34:LEU:HD11  | 3:M:51:LEU:HD21   | 1.95                     | 0.49              |
| 8:V:964:LEU:HD22 | 8:V:1053:LEU:HD22 | 1.94                     | 0.49              |
| 8:V:1057:PHE:HB3 | 8:V:1061:ILE:HG13 | 1.94                     | 0.49              |
| 4:D:94:ALA:HA    | 4:D:97:LEU:HG     | 1.94                     | 0.49              |
| 2:F:34:ILE:HA    | 2:F:37:LEU:HD12   | 1.94                     | 0.49              |
| 7:U:299:LEU:O    | 7:U:303:ARG:HG2   | 2.13                     | 0.49              |
| 7:U:411:TYR:HE1  | 8:V:1033:TYR:CE1  | 2.31                     | 0.49              |
| 7:U:506:TYR:HE1  | 7:U:520:GLN:HG2   | 1.77                     | 0.49              |
| 4:N:51:ILE:HD12  | 4:N:56:MET:HG2    | 1.95                     | 0.49              |
| 1:O:62:ILE:HD13  | 2:P:33:ALA:HB1    | 1.94                     | 0.49              |
| 3:Q:78:ILE:HB    | 4:R:51:ILE:HD12   | 1.95                     | 0.49              |
| 8:V:532:ASP:HA   | 8:V:547:ARG:HH12  | 1.76                     | 0.49              |
| 8:V:887:TRP:CE3  | 8:V:891:GLU:HB3   | 2.47                     | 0.49              |
| 1:A:69:ARG:HB3   | 2:B:25:ASN:OD1    | 2.13                     | 0.49              |
| 5:I:173:DG:N2    | 6:J:143:DT:O2     | 2.45                     | 0.49              |
| 5:I:261:DG:H3'   | 8:V:335:MET:SD    | 2.53                     | 0.49              |
| 3:M:17:ARG:NH2   | 3:M:28:GLY:HA2    | 2.28                     | 0.49              |
| 3:M:64:GLU:OE2   | 8:V:771:ARG:NH1   | 2.46                     | 0.49              |
| 8:V:467:ASN:OD1  | 8:V:469:MET:HB2   | 2.13                     | 0.49              |
| 8:V:807:HIS:CE1  | 8:V:937:ILE:HG12  | 2.48                     | 0.49              |
| 8:V:956:ARG:NH1  | 8:V:960:GLN:HE22  | 2.11                     | 0.49              |
| 7:U:147:TRP:HZ3  | 7:U:443:GLN:HE21  | 1.61                     | 0.48              |
| 7:U:350:LEU:HD21 | 8:V:951:GLU:HB3   | 1.94                     | 0.48              |
| 7:U:464:PHE:CE2  | 7:U:480:LEU:HD11  | 2.47                     | 0.48              |
| 1:O:76:GLN:OE1   | 1:O:80:THR:HA     | 2.13                     | 0.48              |
| 3:C:29:ARG:O     | 3:C:33:LEU:HD23   | 2.13                     | 0.48              |
| 2:F:64:ASN:HA    | 2:F:67:ARG:NH2    | 2.27                     | 0.48              |
| 3:G:45:ALA:O     | 3:G:48:PRO:HD2    | 2.13                     | 0.48              |
| 7:U:176:VAL:HG21 | 7:U:604:PHE:HE1   | 1.79                     | 0.48              |
| 7:U:228:LYS:O    | 7:U:232:ASP:HB2   | 2.13                     | 0.48              |
| 2:L:16:LYS:HB3   | 2:L:19:ARG:HH21   | 1.78                     | 0.48              |
| 2:L:16:LYS:HB3   | 2:L:19:ARG:NH2    | 2.28                     | 0.48              |
| 8:V:118:LEU:HD11 | 8:V:384:TRP:CH2   | 2.48                     | 0.48              |
| 8:V:837:ASP:O    | 8:V:839:LYS:HG2   | 2.13                     | 0.48              |
| 1:A:119:ILE:HD11 | 2:B:46:ILE:HG23   | 1.94                     | 0.48              |
| 2:B:31:LYS:HE2   | 2:B:51:TYR:CZ     | 2.47                     | 0.48              |
| 1:E:46:VAL:O     | 1:E:49:ARG:HB2    | 2.14                     | 0.48              |
| 7:U:162:TYR:HA   | 7:U:613:HIS:CE1   | 2.47                     | 0.48              |
| 7:U:228:LYS:HB2  | 7:U:236:LEU:HG    | 1.95                     | 0.48              |
| 1:K:103:LEU:O    | 1:K:107:THR:HG23  | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:V:827:LYS:HB3   | 8:V:861:SER:O     | 2.13                     | 0.48              |
| 3:C:16:THR:O      | 3:C:20:ARG:HG3    | 2.12                     | 0.48              |
| 3:C:42:ARG:HB2    | 4:D:85:THR:OG1    | 2.13                     | 0.48              |
| 7:U:467:GLN:OE1   | 7:U:472:LYS:HD2   | 2.14                     | 0.48              |
| 7:U:696:TYR:O     | 7:U:700:ARG:N     | 2.35                     | 0.48              |
| 1:K:48:LEU:O      | 1:K:52:ARG:HG3    | 2.14                     | 0.48              |
| 8:V:628:THR:O     | 8:V:631:SER:OG    | 2.30                     | 0.48              |
| 8:V:954:ILE:O     | 8:V:1011:ARG:NH1  | 2.46                     | 0.48              |
| 1:E:99:TYR:O      | 1:E:103:LEU:HG    | 2.13                     | 0.48              |
| 6:J:46:DC:H2''    | 6:J:47:DC:C5      | 2.48                     | 0.48              |
| 7:U:293:LYS:HZ3   | 7:U:377:LYS:HB2   | 1.78                     | 0.48              |
| 7:U:697:ASN:O     | 7:U:701:LYS:HG3   | 2.14                     | 0.48              |
| 2:L:27:GLN:HA     | 2:L:55:ARG:NE     | 2.29                     | 0.48              |
| 4:R:82:LYS:O      | 4:R:83:ARG:NH2    | 2.46                     | 0.48              |
| 8:V:399:LYS:HE2   | 8:V:402:HIS:CD2   | 2.44                     | 0.48              |
| 8:V:1004:LEU:HD23 | 8:V:1014:VAL:HG12 | 1.96                     | 0.48              |
| 4:D:64:ASN:O      | 4:D:68:GLU:OE1    | 2.31                     | 0.48              |
| 5:I:129:DT:H4'    | 5:I:130:DC:OP2    | 2.13                     | 0.48              |
| 6:J:72:DC:H2''    | 6:J:73:DA:H8      | 1.79                     | 0.48              |
| 7:U:142:LEU:HD12  | 7:U:147:TRP:CD1   | 2.49                     | 0.48              |
| 7:U:192:PHE:HB2   | 7:U:196:PHE:CE2   | 2.49                     | 0.48              |
| 7:U:464:PHE:HE2   | 7:U:480:LEU:HD11  | 1.78                     | 0.48              |
| 7:U:645:ASP:O     | 7:U:649:VAL:HG23  | 2.13                     | 0.48              |
| 7:U:729:ASP:HB2   | 7:U:731:LYS:HD2   | 1.95                     | 0.48              |
| 3:M:25:PHE:HB2    | 3:M:56:GLU:OE2    | 2.14                     | 0.48              |
| 1:O:48:LEU:HD11   | 2:P:44:LYS:HE3    | 1.96                     | 0.48              |
| 8:V:118:LEU:HD11  | 8:V:384:TRP:HH2   | 1.78                     | 0.48              |
| 8:V:239:ARG:NH2   | 8:V:270:ASP:O     | 2.47                     | 0.48              |
| 8:V:287:ILE:O     | 8:V:292:LEU:N     | 2.41                     | 0.48              |
| 8:V:824:TRP:NE1   | 8:V:828:LYS:HD2   | 2.29                     | 0.48              |
| 1:A:102:ALA:O     | 1:A:105:GLU:HG3   | 2.13                     | 0.48              |
| 7:U:155:THR:HB    | 7:U:158:PHE:CE1   | 2.49                     | 0.48              |
| 7:U:195:PHE:CE1   | 7:U:406:ILE:HG22  | 2.49                     | 0.48              |
| 7:U:606:HIS:HD2   | 7:U:626:TYR:O     | 1.97                     | 0.48              |
| 1:K:122:LYS:HE2   | 1:O:113:HIS:CE1   | 2.49                     | 0.48              |
| 3:M:30:VAL:HG11   | 3:M:51:LEU:CD1    | 2.33                     | 0.48              |
| 3:M:65:LEU:HB3    | 3:M:86:ALA:HB1    | 1.96                     | 0.48              |
| 3:C:16:THR:O      | 3:C:19:SER:OG     | 2.20                     | 0.48              |
| 3:G:88:ARG:NE     | 3:G:94:ASN:OD1    | 2.32                     | 0.48              |
| 7:U:208:PHE:O     | 7:U:212:LEU:HB2   | 2.14                     | 0.48              |
| 2:L:98:TYR:CE2    | 4:R:62:PHE:HD1    | 2.31                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:M:84:GLN:HE21  | 3:M:88:ARG:HG3   | 1.79                     | 0.48              |
| 4:R:110:GLU:O    | 4:R:113:LYS:HG3  | 2.14                     | 0.48              |
| 8:V:429:LEU:HD11 | 8:V:624:PHE:HB3  | 1.96                     | 0.48              |
| 8:V:817:LEU:O    | 8:V:820:LYS:HB2  | 2.14                     | 0.48              |
| 8:V:962:GLU:O    | 8:V:966:ARG:HG3  | 2.14                     | 0.48              |
| 8:V:973:ASN:O    | 8:V:977:ASP:N    | 2.47                     | 0.48              |
| 2:F:48:GLY:HA2   | 2:F:51:TYR:HE2   | 1.75                     | 0.48              |
| 3:G:70:ALA:HA    | 3:G:82:HIS:NE2   | 2.29                     | 0.48              |
| 5:I:327:DT:H2''  | 5:I:328:DC:C5    | 2.48                     | 0.48              |
| 2:P:64:ASN:HA    | 2:P:67:ARG:NH1   | 2.29                     | 0.48              |
| 8:V:103:GLU:O    | 8:V:106:THR:OG1  | 2.30                     | 0.48              |
| 8:V:322:ILE:HD13 | 8:V:349:LEU:HB3  | 1.96                     | 0.48              |
| 1:A:88:ALA:O     | 1:A:92:LEU:HG    | 2.14                     | 0.47              |
| 1:A:131:ARG:NH1  | 1:A:133:GLU:HB3  | 2.28                     | 0.47              |
| 2:B:71:THR:HA    | 2:B:74:GLU:CD    | 2.39                     | 0.47              |
| 2:F:59:LYS:O     | 2:F:63:GLU:OE1   | 2.32                     | 0.47              |
| 6:J:82:DG:H2'    | 6:J:83:DT:H71    | 1.96                     | 0.47              |
| 7:U:164:VAL:HG23 | 7:U:610:SER:HB2  | 1.96                     | 0.47              |
| 7:U:642:GLU:OE2  | 7:U:646:TYR:OH   | 2.27                     | 0.47              |
| 4:R:76:ARG:O     | 4:R:79:HIS:HB2   | 2.14                     | 0.47              |
| 8:V:333:GLU:HA   | 8:V:338:GLN:HE22 | 1.78                     | 0.47              |
| 8:V:1041:GLU:HA  | 8:V:1044:ARG:HG3 | 1.96                     | 0.47              |
| 4:H:34:TYR:CE2   | 4:H:63:VAL:HB    | 2.48                     | 0.47              |
| 5:I:273:DA:C5    | 5:I:274:DC:C4    | 3.02                     | 0.47              |
| 5:I:279:DT:H2''  | 5:I:280:DA:C8    | 2.49                     | 0.47              |
| 7:U:198:SER:HA   | 7:U:201:GLN:CD   | 2.40                     | 0.47              |
| 7:U:394:ALA:O    | 7:U:397:ASP:HB2  | 2.14                     | 0.47              |
| 7:U:713:TYR:O    | 7:U:717:LEU:HD23 | 2.14                     | 0.47              |
| 2:L:74:GLU:HG2   | 2:L:75:HIS:N     | 2.29                     | 0.47              |
| 3:Q:26:PRO:HG3   | 4:R:37:TYR:CE2   | 2.48                     | 0.47              |
| 8:V:612:ALA:O    | 8:V:617:GLN:NE2  | 2.44                     | 0.47              |
| 8:V:798:MET:C    | 8:V:800:LYS:H    | 2.22                     | 0.47              |
| 7:U:150:VAL:O    | 7:U:152:PRO:HD3  | 2.15                     | 0.47              |
| 4:N:92:GLN:HE22  | 4:N:96:ARG:CZ    | 2.27                     | 0.47              |
| 3:C:88:ARG:NH2   | 3:C:100:VAL:O    | 2.46                     | 0.47              |
| 1:E:52:ARG:O     | 1:E:56:LYS:HG2   | 2.15                     | 0.47              |
| 2:F:90:LEU:HA    | 2:F:93:GLN:NE2   | 2.30                     | 0.47              |
| 3:G:18:SER:O     | 3:G:23:LEU:N     | 2.41                     | 0.47              |
| 5:I:170:DG:H2''  | 5:I:172:DA:H62   | 1.79                     | 0.47              |
| 6:J:0:DC:H2''    | 6:J:1:DT:C6      | 2.49                     | 0.47              |
| 7:U:611:LEU:HD12 | 7:U:612:ALA:N    | 2.30                     | 0.47              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:K:104:PHE:HE2 | 2:L:37:LEU:HB3   | 1.80                     | 0.47              |
| 1:O:116:ARG:NH1 | 1:O:118:THR:O    | 2.46                     | 0.47              |
| 3:Q:78:ILE:HB   | 4:R:51:ILE:CD1   | 2.45                     | 0.47              |
| 8:V:418:GLU:C   | 8:V:420:SER:H    | 2.20                     | 0.47              |
| 8:V:503:LYS:HD2 | 8:V:596:TYR:CZ   | 2.48                     | 0.47              |
| 1:A:90:MET:O    | 1:A:93:GLN:N     | 2.47                     | 0.47              |
| 3:C:97:LEU:HD23 | 3:C:100:VAL:HG11 | 1.97                     | 0.47              |
| 6:J:50:DT:C4    | 6:J:51:DT:C4     | 3.03                     | 0.47              |
| 6:J:61:DA:OP1   | 2:L:36:ARG:NH2   | 2.47                     | 0.47              |
| 6:J:159:DC:H1'  | 6:J:160:DG:C4    | 2.50                     | 0.47              |
| 7:U:398:TRP:HD1 | 7:U:402:HIS:CE1  | 2.32                     | 0.47              |
| 2:L:92:ARG:NE   | 2:L:92:ARG:HA    | 2.29                     | 0.47              |
| 1:O:72:ARG:HG2  | 1:O:84:PHE:CE2   | 2.50                     | 0.47              |
| 4:R:36:ILE:HG13 | 4:R:37:TYR:N     | 2.28                     | 0.47              |
| 8:V:107:LYS:NZ  | 8:V:214:LYS:HG3  | 2.30                     | 0.47              |
| 8:V:799:PRO:HG3 | 8:V:822:ARG:HE   | 1.80                     | 0.47              |
| 8:V:949:ASN:HA  | 8:V:952:GLU:CD   | 2.40                     | 0.47              |
| 8:V:1026:PRO:HA | 8:V:1029:GLU:OE1 | 2.13                     | 0.47              |
| 3:G:25:PHE:CE1  | 3:G:56:GLU:HG2   | 2.50                     | 0.47              |
| 8:V:122:PHE:HE2 | 8:V:375:PHE:HA   | 1.78                     | 0.47              |
| 8:V:385:PHE:HZ  | 8:V:398:VAL:HG12 | 1.80                     | 0.47              |
| 2:B:74:GLU:HG2  | 2:B:75:HIS:N     | 2.30                     | 0.47              |
| 3:C:50:TYR:OH   | 4:D:108:VAL:HA   | 2.14                     | 0.47              |
| 5:I:131:DA:C4   | 5:I:132:DG:C5    | 3.03                     | 0.47              |
| 5:I:262:DC:P    | 8:V:335:MET:H    | 2.37                     | 0.47              |
| 6:J:27:DC:H2''  | 6:J:28:DT:C4     | 2.49                     | 0.47              |
| 6:J:52:DG:H1'   | 6:J:53:DG:C8     | 2.50                     | 0.47              |
| 6:J:131:DG:C5   | 6:J:132:DC:C4    | 3.02                     | 0.47              |
| 7:U:436:GLY:HA2 | 7:U:709:PHE:HZ   | 1.79                     | 0.47              |
| 7:U:607:ASP:OD1 | 7:U:609:PRO:HD2  | 2.13                     | 0.47              |
| 3:M:29:ARG:NE   | 4:N:32:GLU:OE2   | 2.47                     | 0.47              |
| 4:N:114:ALA:O   | 4:N:118:TYR:N    | 2.33                     | 0.47              |
| 4:R:41:VAL:HA   | 4:R:44:GLN:HG3   | 1.96                     | 0.47              |
| 4:R:81:ASN:O    | 4:R:83:ARG:NH1   | 2.46                     | 0.47              |
| 8:V:551:SER:H   | 8:V:557:ARG:NH2  | 2.11                     | 0.47              |
| 8:V:820:LYS:HB3 | 8:V:872:GLU:OE1  | 2.14                     | 0.47              |
| 1:E:116:ARG:HD2 | 1:E:120:MET:HE1  | 1.97                     | 0.47              |
| 5:I:325:DG:C2   | 6:J:-9:DA:C2     | 3.02                     | 0.47              |
| 5:I:329:DA:H2'' | 5:I:330:DT:C6    | 2.50                     | 0.47              |
| 6:J:3:DA:C2'    | 6:J:4:DG:C8      | 2.98                     | 0.47              |
| 7:U:293:LYS:NZ  | 7:U:377:LYS:HB2  | 2.30                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:U:303:ARG:HA   | 7:U:370:LEU:HD21 | 1.97                     | 0.47              |
| 3:M:115:LEU:HD22 | 2:P:44:LYS:HD3   | 1.97                     | 0.47              |
| 8:V:807:HIS:NE2  | 8:V:937:ILE:HG23 | 2.30                     | 0.47              |
| 8:V:918:LYS:HG3  | 8:V:919:THR:H    | 1.79                     | 0.47              |
| 8:V:955:LYS:O    | 8:V:958:LYS:N    | 2.48                     | 0.47              |
| 3:C:91:GLU:C     | 3:C:95:LYS:HZ3   | 2.23                     | 0.47              |
| 4:D:99:LEU:HB2   | 4:D:104:ALA:HB2  | 1.96                     | 0.47              |
| 7:U:494:VAL:O    | 7:U:498:LYS:N    | 2.47                     | 0.47              |
| 3:M:81:ARG:CZ    | 3:M:85:LEU:HD21  | 2.45                     | 0.47              |
| 4:R:43:LYS:HA    | 4:R:47:PRO:HA    | 1.96                     | 0.47              |
| 5:I:275:DT:H2''  | 5:I:276:DC:C6    | 2.50                     | 0.47              |
| 6:J:26:DC:H2''   | 6:J:27:DC:C6     | 2.49                     | 0.47              |
| 7:U:467:GLN:O    | 7:U:472:LYS:HG2  | 2.15                     | 0.47              |
| 1:K:54:TYR:HB3   | 2:L:40:ARG:HB2   | 1.95                     | 0.47              |
| 1:O:59:GLU:CD    | 1:O:60:LEU:N     | 2.73                     | 0.47              |
| 8:V:439:LYS:HB3  | 8:V:443:LYS:NZ   | 2.30                     | 0.47              |
| 8:V:521:VAL:HA   | 8:V:592:VAL:HG23 | 1.96                     | 0.47              |
| 8:V:614:ARG:NH2  | 10:V:1202:BEF:F2 | 2.38                     | 0.47              |
| 1:A:113:HIS:CE1  | 1:E:122:LYS:HB3  | 2.45                     | 0.46              |
| 3:C:14:ALA:HA    | 6:J:199:DG:H5'   | 1.97                     | 0.46              |
| 3:G:31:HIS:HD2   | 3:G:35:ARG:NH1   | 2.11                     | 0.46              |
| 3:G:83:LEU:O     | 3:G:87:VAL:HG22  | 2.15                     | 0.46              |
| 5:I:102:DG:H2''  | 5:I:103:DA:H8    | 1.80                     | 0.46              |
| 5:I:197:DA:H3'   | 3:Q:28:GLY:HA3   | 1.97                     | 0.46              |
| 5:I:308:DA:C2    | 6:J:8:DG:C2      | 3.04                     | 0.46              |
| 6:J:239:DC:H2''  | 6:J:240:DA:OP2   | 2.15                     | 0.46              |
| 7:U:444:PHE:HE2  | 7:U:502:LEU:HD11 | 1.79                     | 0.46              |
| 7:U:738:ARG:HA   | 7:U:741:GLN:HG2  | 1.96                     | 0.46              |
| 1:K:67:PHE:O     | 1:K:70:LEU:HB2   | 2.15                     | 0.46              |
| 8:V:414:LYS:HD2  | 8:V:613:HIS:CE1  | 2.50                     | 0.46              |
| 1:A:93:GLN:O     | 1:A:96:SER:N     | 2.47                     | 0.46              |
| 3:C:90:ASP:HB3   | 3:C:93:LEU:HB2   | 1.97                     | 0.46              |
| 4:D:36:ILE:HG13  | 4:D:37:TYR:N     | 2.30                     | 0.46              |
| 5:I:165:DG:C6    | 5:I:166:DA:C2    | 3.02                     | 0.46              |
| 6:J:47:DC:H4'    | 6:J:48:DC:H5'    | 1.97                     | 0.46              |
| 6:J:173:DA:H2''  | 6:J:174:DT:H5'   | 1.97                     | 0.46              |
| 7:U:311:TYR:CE2  | 7:U:362:PRO:HB3  | 2.50                     | 0.46              |
| 7:U:334:GLU:N    | 7:U:354:ILE:O    | 2.46                     | 0.46              |
| 7:U:382:ALA:C    | 7:U:383:LEU:HD12 | 2.40                     | 0.46              |
| 7:U:434:ILE:HG23 | 7:U:435:GLU:HG3  | 1.96                     | 0.46              |
| 7:U:613:HIS:HB3  | 7:U:617:ARG:NE   | 2.28                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:U:738:ARG:HA   | 7:U:741:GLN:CG   | 2.44                     | 0.46              |
| 2:L:84:MET:HE2   | 2:L:88:TYR:HE2   | 1.79                     | 0.46              |
| 1:O:74:ILE:HG22  | 2:P:66:ILE:HG21  | 1.97                     | 0.46              |
| 5:I:33:DG:C2     | 5:I:34:DG:C4     | 3.03                     | 0.46              |
| 5:I:81:DC:C2     | 6:J:234:DG:N2    | 2.72                     | 0.46              |
| 5:I:161:DG:H2''  | 5:I:162:DC:O5'   | 2.15                     | 0.46              |
| 2:L:46:ILE:HG22  | 2:L:47:SER:O     | 2.15                     | 0.46              |
| 2:L:96:THR:O     | 3:Q:101:THR:HG22 | 2.15                     | 0.46              |
| 4:N:36:ILE:HG13  | 4:N:37:TYR:N     | 2.30                     | 0.46              |
| 1:O:62:ILE:HD12  | 2:P:29:ILE:HG23  | 1.98                     | 0.46              |
| 8:V:225:LEU:HD21 | 8:V:414:LYS:HA   | 1.98                     | 0.46              |
| 8:V:337:SER:HB2  | 8:V:369:PHE:CZ   | 2.50                     | 0.46              |
| 8:V:464:ARG:HD2  | 8:V:466:LEU:HG   | 1.97                     | 0.46              |
| 8:V:594:VAL:HG12 | 8:V:624:PHE:HB2  | 1.97                     | 0.46              |
| 8:V:797:ARG:HD3  | 8:V:831:TYR:HD2  | 1.79                     | 0.46              |
| 3:C:113:SER:HA   | 3:C:116:LEU:HD23 | 1.97                     | 0.46              |
| 7:U:589:LEU:HD21 | 7:U:720:PHE:CD1  | 2.50                     | 0.46              |
| 2:L:34:ILE:HG21  | 2:L:51:TYR:HD1   | 1.81                     | 0.46              |
| 8:V:443:LYS:HG2  | 8:V:448:ASP:HB2  | 1.96                     | 0.46              |
| 8:V:824:TRP:CE3  | 8:V:827:LYS:HD3  | 2.51                     | 0.46              |
| 6:J:269:DA:H8    | 6:J:269:DA:OP2   | 1.99                     | 0.46              |
| 7:U:475:ASP:O    | 7:U:479:LYS:HB2  | 2.15                     | 0.46              |
| 1:K:122:LYS:HG3  | 1:O:113:HIS:CE1  | 2.39                     | 0.46              |
| 2:L:15:ALA:HA    | 2:L:17:ARG:NH1   | 2.30                     | 0.46              |
| 2:L:84:MET:O     | 2:L:87:VAL:HB    | 2.16                     | 0.46              |
| 3:Q:73:ASN:OD1   | 3:Q:75:LYS:HG2   | 2.15                     | 0.46              |
| 8:V:549:ASP:OD1  | 8:V:550:GLY:N    | 2.48                     | 0.46              |
| 8:V:817:LEU:HA   | 8:V:820:LYS:HG2  | 1.97                     | 0.46              |
| 8:V:976:PHE:HA   | 8:V:998:ARG:HH21 | 1.81                     | 0.46              |
| 2:B:84:MET:H     | 2:B:84:MET:HG3   | 1.47                     | 0.46              |
| 4:D:62:PHE:O     | 4:D:66:VAL:HG23  | 2.16                     | 0.46              |
| 6:J:24:DT:H2''   | 6:J:25:DG:H8     | 1.81                     | 0.46              |
| 7:U:173:MET:HG2  | 7:U:628:TYR:HB3  | 1.97                     | 0.46              |
| 7:U:338:GLN:OE1  | 8:V:907:ILE:N    | 2.48                     | 0.46              |
| 7:U:342:VAL:HG13 | 8:V:931:TRP:CZ3  | 2.50                     | 0.46              |
| 2:L:32:PRO:O     | 2:L:36:ARG:HG3   | 2.15                     | 0.46              |
| 1:O:126:LEU:O    | 1:O:130:ILE:HG12 | 2.16                     | 0.46              |
| 3:Q:23:LEU:HG    | 3:Q:25:PHE:H     | 1.81                     | 0.46              |
| 4:R:83:ARG:NE    | 4:R:83:ARG:HA    | 2.30                     | 0.46              |
| 8:V:440:TRP:O    | 8:V:444:ILE:HG13 | 2.16                     | 0.46              |
| 8:V:636:ILE:O    | 8:V:640:ALA:N    | 2.36                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:V:854:LYS:HZ3  | 8:V:858:LEU:HD12 | 1.80                     | 0.46              |
| 8:V:928:LYS:HA   | 8:V:928:LYS:HD2  | 1.63                     | 0.46              |
| 1:A:100:LEU:HD21 | 2:B:58:LEU:HD13  | 1.97                     | 0.46              |
| 6:J:151:DG:C2    | 6:J:152:DA:N6    | 2.84                     | 0.46              |
| 7:U:149:SER:C    | 7:U:151:ILE:H    | 2.22                     | 0.46              |
| 7:U:734:LYS:O    | 7:U:738:ARG:HD3  | 2.16                     | 0.46              |
| 3:M:58:LEU:HD12  | 3:M:59:THR:N     | 2.31                     | 0.46              |
| 4:N:92:GLN:HE22  | 4:N:96:ARG:NH2   | 2.14                     | 0.46              |
| 8:V:203:GLY:O    | 8:V:207:LEU:HG   | 2.16                     | 0.46              |
| 8:V:809:LEU:O    | 8:V:936:ARG:NH2  | 2.49                     | 0.46              |
| 8:V:893:ARG:O    | 8:V:897:THR:OG1  | 2.29                     | 0.46              |
| 2:B:91:LYS:HE2   | 2:B:91:LYS:HB3   | 1.46                     | 0.46              |
| 3:G:26:PRO:HG2   | 3:G:29:ARG:HB3   | 1.98                     | 0.46              |
| 4:H:111:GLY:O    | 4:H:115:VAL:HG22 | 2.15                     | 0.46              |
| 7:U:307:ARG:HD3  | 7:U:362:PRO:HG2  | 1.98                     | 0.46              |
| 7:U:386:MET:O    | 7:U:390:VAL:HG23 | 2.16                     | 0.46              |
| 7:U:653:ASP:O    | 7:U:656:LYS:HB3  | 2.16                     | 0.46              |
| 7:U:716:ILE:HG23 | 7:U:717:LEU:HD22 | 1.97                     | 0.46              |
| 1:K:107:THR:HG22 | 1:K:124:ILE:HA   | 1.97                     | 0.46              |
| 8:V:278:GLY:O    | 8:V:283:ARG:NH1  | 2.49                     | 0.46              |
| 8:V:797:ARG:CZ   | 8:V:825:THR:HG21 | 2.46                     | 0.46              |
| 3:C:57:TYR:O     | 3:C:61:GLU:HG2   | 2.15                     | 0.46              |
| 5:I:4:DG:H2"     | 5:I:5:DA:C8      | 2.51                     | 0.46              |
| 1:K:63:ARG:HB3   | 1:K:66:PRO:HD2   | 1.98                     | 0.46              |
| 3:M:51:LEU:O     | 3:M:55:LEU:HG    | 2.16                     | 0.46              |
| 2:P:75:HIS:HD2   | 4:R:89:ARG:NH1   | 2.14                     | 0.46              |
| 3:Q:66:ALA:HB1   | 3:Q:78:ILE:HG21  | 1.97                     | 0.46              |
| 4:R:42:LEU:O     | 4:R:46:HIS:N     | 2.48                     | 0.46              |
| 4:R:49:THR:HG22  | 4:R:50:GLY:O     | 2.16                     | 0.46              |
| 8:V:185:PHE:CD2  | 8:V:237:TYR:HE1  | 2.33                     | 0.46              |
| 8:V:850:GLU:O    | 8:V:854:LYS:HB3  | 2.15                     | 0.46              |
| 5:I:33:DG:H2"    | 5:I:34:DG:H8     | 1.80                     | 0.46              |
| 5:I:72:DC:H2"    | 5:I:73:DG:H8     | 1.80                     | 0.46              |
| 5:I:163:DT:H2"   | 5:I:164:DC:C6    | 2.51                     | 0.46              |
| 6:J:151:DG:C2    | 6:J:152:DA:C6    | 3.04                     | 0.46              |
| 7:U:632:HIS:NE2  | 7:U:633:ASP:OD2  | 2.49                     | 0.46              |
| 3:Q:80:PRO:HA    | 3:Q:83:LEU:HB2   | 1.98                     | 0.46              |
| 8:V:425:LYS:NZ   | 8:V:622:LYS:HE2  | 2.31                     | 0.46              |
| 8:V:981:LYS:HD3  | 8:V:984:PRO:HG3  | 1.98                     | 0.46              |
| 1:A:112:ILE:HG13 | 1:A:113:HIS:N    | 2.31                     | 0.45              |
| 2:B:50:ILE:O     | 2:B:54:THR:HG23  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:102:ALA:HA   | 1:E:105:GLU:HG2  | 1.97                     | 0.45              |
| 5:I:273:DA:N6    | 6:J:43:DA:N6     | 2.65                     | 0.45              |
| 6:J:51:DT:H2"    | 6:J:52:DG:C8     | 2.51                     | 0.45              |
| 7:U:214:LEU:CD1  | 7:U:222:SER:HB2  | 2.46                     | 0.45              |
| 7:U:426:THR:O    | 7:U:534:ARG:HB3  | 2.16                     | 0.45              |
| 7:U:477:SER:HB3  | 7:U:478:ARG:NH2  | 2.30                     | 0.45              |
| 2:L:47:SER:HB3   | 2:L:50:ILE:HG12  | 1.97                     | 0.45              |
| 3:M:95:LYS:CE    | 4:N:100:PRO:HG3  | 2.46                     | 0.45              |
| 4:N:42:LEU:O     | 4:N:46:HIS:N     | 2.48                     | 0.45              |
| 1:O:60:LEU:HD13  | 1:O:93:GLN:NE2   | 2.30                     | 0.45              |
| 1:O:99:TYR:HD1   | 2:P:95:ARG:NH1   | 2.14                     | 0.45              |
| 4:R:94:ALA:HA    | 4:R:97:LEU:HB2   | 1.97                     | 0.45              |
| 8:V:243:LYS:HG3  | 8:V:243:LYS:O    | 2.16                     | 0.45              |
| 8:V:823:MET:HG3  | 8:V:864:ASN:ND2  | 2.32                     | 0.45              |
| 8:V:887:TRP:HA   | 8:V:891:GLU:CB   | 2.46                     | 0.45              |
| 3:C:51:LEU:O     | 3:C:55:LEU:HG    | 2.16                     | 0.45              |
| 1:E:121:PRO:O    | 1:E:124:ILE:HG22 | 2.16                     | 0.45              |
| 6:J:-5:DT:H2"    | 6:J:-4:DT:C6     | 2.51                     | 0.45              |
| 6:J:12:DA:C5     | 6:J:13:DT:C4     | 3.04                     | 0.45              |
| 7:U:137:GLN:O    | 7:U:457:ILE:HG13 | 2.17                     | 0.45              |
| 7:U:180:GLY:HA2  | 7:U:183:ILE:CG1  | 2.46                     | 0.45              |
| 7:U:205:PHE:CD1  | 7:U:602:LYS:HD3  | 2.51                     | 0.45              |
| 7:U:285:GLU:O    | 7:U:289:SER:N    | 2.49                     | 0.45              |
| 7:U:411:TYR:OH   | 8:V:1036:SER:HB2 | 2.15                     | 0.45              |
| 7:U:441:ILE:HB   | 7:U:503:PHE:HZ   | 1.81                     | 0.45              |
| 3:Q:30:VAL:HG12  | 3:Q:34:LEU:HG    | 1.98                     | 0.45              |
| 2:B:31:LYS:HE2   | 2:B:51:TYR:OH    | 2.16                     | 0.45              |
| 2:B:70:VAL:O     | 2:B:74:GLU:OE1   | 2.34                     | 0.45              |
| 3:C:62:ILE:HG13  | 3:C:63:LEU:N     | 2.32                     | 0.45              |
| 1:E:65:LEU:HD23  | 1:E:65:LEU:HA    | 1.78                     | 0.45              |
| 1:E:67:PHE:O     | 1:E:71:VAL:HG23  | 2.15                     | 0.45              |
| 3:G:92:GLU:O     | 3:G:95:LYS:HG2   | 2.16                     | 0.45              |
| 5:I:249:DC:H5"   | 2:L:45:ARG:HD2   | 1.97                     | 0.45              |
| 5:I:258:DA:C2'   | 1:K:65:LEU:HD12  | 2.46                     | 0.45              |
| 6:J:117:DA:C2    | 6:J:118:DT:C2    | 3.05                     | 0.45              |
| 7:U:331:ALA:N    | 7:U:356:THR:OG1  | 2.48                     | 0.45              |
| 7:U:548:ASP:O    | 7:U:606:HIS:N    | 2.32                     | 0.45              |
| 3:M:39:TYR:CZ    | 4:N:71:ALA:HB1   | 2.52                     | 0.45              |
| 3:Q:44:GLY:N     | 4:R:86:ILE:O     | 2.36                     | 0.45              |
| 8:V:496:HIS:HA   | 8:V:499:TYR:HB3  | 1.98                     | 0.45              |
| 8:V:809:LEU:HD12 | 8:V:933:ASN:HB2  | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:J:101:DG:H1'   | 6:J:102:DA:C8    | 2.51                     | 0.45              |
| 6:J:113:DA:C5    | 6:J:114:DC:C4    | 3.04                     | 0.45              |
| 7:U:333:PHE:HD2  | 7:U:354:ILE:HG13 | 1.80                     | 0.45              |
| 7:U:576:LEU:O    | 7:U:580:LYS:HG3  | 2.17                     | 0.45              |
| 2:L:99:GLY:O     | 2:L:100:PHE:HD2  | 1.99                     | 0.45              |
| 3:M:57:TYR:HB2   | 4:N:110:GLU:OE2  | 2.16                     | 0.45              |
| 4:N:62:PHE:HD1   | 2:P:98:TYR:HE2   | 1.64                     | 0.45              |
| 3:Q:79:ILE:HG13  | 3:Q:82:HIS:H     | 1.81                     | 0.45              |
| 8:V:101:ASP:O    | 8:V:105:THR:N    | 2.42                     | 0.45              |
| 5:I:83:DG:C5     | 5:I:84:DC:C4     | 3.05                     | 0.45              |
| 6:J:54:DC:H2''   | 6:J:55:DG:C8     | 2.51                     | 0.45              |
| 7:U:691:PRO:O    | 7:U:696:TYR:HE2  | 1.99                     | 0.45              |
| 1:O:60:LEU:HD21  | 1:O:90:MET:HE1   | 1.98                     | 0.45              |
| 1:O:124:ILE:O    | 1:O:128:ARG:HG3  | 2.17                     | 0.45              |
| 8:V:357:GLN:HA   | 8:V:603:GLN:NE2  | 2.31                     | 0.45              |
| 5:I:172:DA:H2''  | 5:I:173:DG:H8    | 1.79                     | 0.45              |
| 6:J:61:DA:P      | 2:L:36:ARG:HH12  | 2.39                     | 0.45              |
| 7:U:266:PHE:O    | 7:U:268:GLU:N    | 2.46                     | 0.45              |
| 7:U:346:HIS:CB   | 8:V:905:ASN:HD21 | 2.30                     | 0.45              |
| 7:U:411:TYR:CE1  | 8:V:1033:TYR:CD1 | 3.01                     | 0.45              |
| 3:M:90:ASP:OD2   | 3:M:93:LEU:HD13  | 2.16                     | 0.45              |
| 1:A:70:LEU:HD21  | 2:B:26:ILE:N     | 2.32                     | 0.45              |
| 1:E:97:GLU:HA    | 1:E:100:LEU:HG   | 1.98                     | 0.45              |
| 3:G:79:ILE:HG22  | 4:H:52:SER:OG    | 2.16                     | 0.45              |
| 5:I:123:DC:H2''  | 5:I:124:DA:H8    | 1.81                     | 0.45              |
| 6:J:3:DA:H2''    | 6:J:4:DG:H8      | 1.78                     | 0.45              |
| 7:U:530:LEU:HD23 | 7:U:530:LEU:H    | 1.82                     | 0.45              |
| 7:U:734:LYS:NZ   | 7:U:735:ARG:HH21 | 2.14                     | 0.45              |
| 3:Q:42:ARG:HB2   | 4:R:85:THR:OG1   | 2.16                     | 0.45              |
| 8:V:437:GLN:OE1  | 8:V:479:PRO:HG3  | 2.17                     | 0.45              |
| 8:V:994:GLU:O    | 8:V:997:ASP:N    | 2.50                     | 0.45              |
| 1:A:83:ARG:HG2   | 6:J:218:DT:H5'   | 1.99                     | 0.45              |
| 7:U:342:VAL:HG13 | 8:V:931:TRP:HZ3  | 1.81                     | 0.45              |
| 7:U:458:ARG:HH12 | 7:U:479:LYS:NZ   | 2.15                     | 0.45              |
| 7:U:581:ASN:OD1  | 7:U:583:GLU:HG3  | 2.17                     | 0.45              |
| 3:M:48:PRO:O     | 3:M:51:LEU:HG    | 2.16                     | 0.45              |
| 8:V:433:MET:HB2  | 8:V:628:THR:CG2  | 2.46                     | 0.45              |
| 8:V:926:TYR:O    | 8:V:930:PHE:HB2  | 2.16                     | 0.45              |
| 8:V:1055:LYS:HA  | 8:V:1058:ASN:OD1 | 2.17                     | 0.45              |
| 3:C:17:ARG:O     | 3:C:20:ARG:HB2   | 2.17                     | 0.45              |
| 4:H:96:ARG:HG2   | 4:H:96:ARG:NH1   | 2.32                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:I:70:DC:H2''   | 5:I:71:DG:C8     | 2.52                     | 0.45              |
| 5:I:307:DC:H2''  | 5:I:308:DA:C8    | 2.52                     | 0.45              |
| 7:U:135:HIS:ND1  | 7:U:136:GLU:OE1  | 2.50                     | 0.45              |
| 7:U:159:LYS:HZ2  | 7:U:545:HIS:H    | 1.65                     | 0.45              |
| 7:U:215:TYR:CD2  | 7:U:226:ILE:HG12 | 2.52                     | 0.45              |
| 7:U:283:THR:OG1  | 7:U:285:GLU:OE1  | 2.34                     | 0.45              |
| 7:U:384:LYS:NZ   | 7:U:386:MET:SD   | 2.87                     | 0.45              |
| 7:U:699:ALA:O    | 7:U:703:LEU:HG   | 2.17                     | 0.45              |
| 1:K:111:ALA:O    | 1:K:115:LYS:N    | 2.50                     | 0.45              |
| 8:V:131:PRO:HG2  | 8:V:133:PHE:HD2  | 1.82                     | 0.45              |
| 8:V:494:ASP:HA   | 8:V:540:PHE:CE1  | 2.52                     | 0.45              |
| 1:E:116:ARG:NH1  | 1:E:118:THR:O    | 2.50                     | 0.45              |
| 7:U:148:THR:H    | 7:U:431:ARG:HH22 | 1.63                     | 0.45              |
| 7:U:155:THR:H    | 7:U:427:GLN:NE2  | 2.15                     | 0.45              |
| 7:U:454:ARG:NH1  | 7:U:516:GLU:OE2  | 2.50                     | 0.45              |
| 7:U:602:LYS:HE3  | 7:U:629:GLU:HG3  | 1.98                     | 0.45              |
| 2:L:31:LYS:HA    | 2:L:34:ILE:HD12  | 1.98                     | 0.45              |
| 3:Q:61:GLU:O     | 3:Q:64:GLU:HG3   | 2.16                     | 0.45              |
| 4:R:87:THR:O     | 4:R:91:ILE:HG12  | 2.16                     | 0.45              |
| 8:V:809:LEU:HB3  | 8:V:936:ARG:NH2  | 2.31                     | 0.45              |
| 8:V:833:PRO:HG2  | 8:V:857:LEU:O    | 2.17                     | 0.45              |
| 8:V:976:PHE:HA   | 8:V:998:ARG:NH2  | 2.32                     | 0.45              |
| 5:I:102:DG:C4    | 5:I:103:DA:N7    | 2.85                     | 0.44              |
| 5:I:188:DG:H2''  | 5:I:189:DG:C8    | 2.52                     | 0.44              |
| 6:J:54:DC:H1'    | 8:V:579:ARG:HH21 | 1.83                     | 0.44              |
| 7:U:215:TYR:HD2  | 7:U:226:ILE:HG23 | 1.82                     | 0.44              |
| 7:U:510:VAL:HG22 | 7:U:520:GLN:CD   | 2.43                     | 0.44              |
| 7:U:521:PRO:O    | 7:U:522:LEU:HD23 | 2.17                     | 0.44              |
| 1:K:121:PRO:HG3  | 2:L:50:ILE:HD13  | 1.99                     | 0.44              |
| 2:L:67:ARG:O     | 2:L:71:THR:OG1   | 2.24                     | 0.44              |
| 8:V:357:GLN:HA   | 8:V:603:GLN:CD   | 2.42                     | 0.44              |
| 8:V:824:TRP:HE3  | 8:V:827:LYS:HD3  | 1.81                     | 0.44              |
| 8:V:910:ILE:HG13 | 8:V:914:LEU:HD12 | 1.99                     | 0.44              |
| 8:V:967:LYS:HE2  | 8:V:1057:PHE:CZ  | 2.52                     | 0.44              |
| 1:A:118:THR:HA   | 2:B:45:ARG:HB3   | 1.99                     | 0.44              |
| 3:C:59:THR:O     | 3:C:63:LEU:HD23  | 2.16                     | 0.44              |
| 1:E:85:GLN:NE2   | 2:F:82:THR:HA    | 2.31                     | 0.44              |
| 6:J:9:DT:H2''    | 6:J:10:DA:H8     | 1.81                     | 0.44              |
| 6:J:145:DC:H6    | 6:J:145:DC:H2'   | 1.56                     | 0.44              |
| 1:K:46:VAL:HG22  | 1:K:49:ARG:NH2   | 2.32                     | 0.44              |
| 1:K:108:ASN:ND2  | 2:L:42:GLY:O     | 2.51                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:V:394:GLN:HG2  | 8:V:396:LYS:HB2  | 2.00                     | 0.44              |
| 8:V:652:GLN:OE1  | 8:V:655:ARG:NH2  | 2.50                     | 0.44              |
| 8:V:820:LYS:HZ2  | 8:V:866:GLN:HE21 | 1.65                     | 0.44              |
| 8:V:996:GLU:HA   | 8:V:1028:PHE:HZ  | 1.81                     | 0.44              |
| 8:V:1055:LYS:HA  | 8:V:1058:ASN:CG  | 2.43                     | 0.44              |
| 2:F:90:LEU:HD13  | 2:F:95:ARG:O     | 2.16                     | 0.44              |
| 5:I:257:DA:H2    | 6:J:58:DT:H3     | 1.65                     | 0.44              |
| 7:U:594:GLY:O    | 7:U:597:MET:HB2  | 2.18                     | 0.44              |
| 7:U:646:TYR:CE2  | 7:U:679:THR:HG21 | 2.53                     | 0.44              |
| 3:M:77:ARG:HA    | 4:N:50:GLY:C     | 2.43                     | 0.44              |
| 8:V:313:LEU:HD22 | 8:V:318:TRP:CZ2  | 2.49                     | 0.44              |
| 8:V:541:ARG:NH2  | 8:V:543:TYR:OH   | 2.44                     | 0.44              |
| 8:V:605:ASP:O    | 8:V:609:MET:HG2  | 2.18                     | 0.44              |
| 8:V:824:TRP:CE3  | 8:V:867:PRO:HB3  | 2.52                     | 0.44              |
| 3:C:30:VAL:O     | 3:C:34:LEU:HG    | 2.17                     | 0.44              |
| 1:E:97:GLU:HA    | 1:E:100:LEU:CD2  | 2.47                     | 0.44              |
| 2:F:78:ARG:HG3   | 2:F:80:THR:H     | 1.82                     | 0.44              |
| 7:U:153:LEU:HD23 | 7:U:153:LEU:H    | 1.82                     | 0.44              |
| 7:U:250:CYS:HB3  | 7:U:254:MET:HE1  | 1.98                     | 0.44              |
| 7:U:391:LEU:HD12 | 7:U:392:LEU:N    | 2.32                     | 0.44              |
| 7:U:644:LEU:O    | 7:U:648:ILE:HG13 | 2.17                     | 0.44              |
| 1:K:97:GLU:CD    | 1:K:98:ALA:N     | 2.75                     | 0.44              |
| 2:L:16:LYS:HE3   | 2:L:19:ARG:CD    | 2.48                     | 0.44              |
| 2:L:77:LYS:O     | 2:L:78:ARG:HD2   | 2.16                     | 0.44              |
| 4:N:52:SER:O     | 4:N:56:MET:HG3   | 2.18                     | 0.44              |
| 3:Q:18:SER:O     | 3:Q:23:LEU:N     | 2.37                     | 0.44              |
| 1:A:126:LEU:O    | 1:A:129:ARG:HB2  | 2.17                     | 0.44              |
| 2:B:23:ARG:NE    | 2:B:24:ASP:OD2   | 2.51                     | 0.44              |
| 3:C:97:LEU:HD21  | 4:D:62:PHE:CE1   | 2.53                     | 0.44              |
| 4:D:105:LYS:O    | 4:D:108:VAL:HG12 | 2.18                     | 0.44              |
| 2:F:30:THR:HB    | 2:F:32:PRO:HD2   | 2.00                     | 0.44              |
| 2:F:64:ASN:HA    | 2:F:67:ARG:NH1   | 2.33                     | 0.44              |
| 3:G:31:HIS:O     | 3:G:35:ARG:HG3   | 2.17                     | 0.44              |
| 3:G:71:ARG:HG2   | 3:G:71:ARG:HH11  | 1.82                     | 0.44              |
| 7:U:347:PRO:HD2  | 8:V:1068:LYS:NZ  | 2.33                     | 0.44              |
| 4:R:110:GLU:OE1  | 4:R:110:GLU:HA   | 2.17                     | 0.44              |
| 8:V:886:ASN:OD1  | 8:V:886:ASN:N    | 2.49                     | 0.44              |
| 8:V:1022:ILE:CG2 | 8:V:1034:PHE:HB3 | 2.48                     | 0.44              |
| 1:A:65:LEU:HD23  | 1:A:65:LEU:HA    | 1.76                     | 0.44              |
| 6:J:113:DA:H5''  | 3:Q:42:ARG:HG2   | 1.98                     | 0.44              |
| 7:U:215:TYR:CD2  | 7:U:226:ILE:HG23 | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:U:650:LYS:O    | 7:U:652:GLN:N    | 2.50                     | 0.44              |
| 7:U:682:ASN:HD22 | 7:U:689:PRO:HD3  | 1.83                     | 0.44              |
| 8:V:211:HIS:CD2  | 8:V:346:ARG:HH12 | 2.36                     | 0.44              |
| 8:V:327:HIS:HB3  | 8:V:330:LYS:NZ   | 2.33                     | 0.44              |
| 1:A:48:LEU:HB3   | 1:A:52:ARG:HH12  | 1.83                     | 0.44              |
| 3:C:84:GLN:HA    | 3:C:87:VAL:HG12  | 2.00                     | 0.44              |
| 1:E:46:VAL:O     | 1:E:50:GLU:OE1   | 2.35                     | 0.44              |
| 3:G:67:GLY:HA2   | 3:G:78:ILE:HD11  | 1.99                     | 0.44              |
| 6:J:-14:DT:H2''  | 6:J:-13:DG:C8    | 2.53                     | 0.44              |
| 7:U:508:LYS:O    | 7:U:511:PRO:HD2  | 2.17                     | 0.44              |
| 7:U:563:MET:HE3  | 7:U:592:ASN:HB2  | 2.00                     | 0.44              |
| 3:M:21:ALA:O     | 4:N:117:LYS:HD3  | 2.18                     | 0.44              |
| 1:O:124:ILE:O    | 1:O:128:ARG:N    | 2.37                     | 0.44              |
| 2:P:60:VAL:HA    | 2:P:63:GLU:HG2   | 1.99                     | 0.44              |
| 8:V:273:ALA:HA   | 8:V:298:VAL:O    | 2.17                     | 0.44              |
| 8:V:276:LEU:O    | 8:V:305:ILE:HD13 | 2.18                     | 0.44              |
| 8:V:820:LYS:HD3  | 8:V:820:LYS:HA   | 1.74                     | 0.44              |
| 1:A:122:LYS:O    | 1:A:125:GLN:HG3  | 2.18                     | 0.44              |
| 1:E:100:LEU:HD13 | 1:E:104:PHE:HE2  | 1.83                     | 0.44              |
| 5:I:280:DA:H2''  | 5:I:281:DG:C8    | 2.52                     | 0.44              |
| 6:J:130:DG:H1'   | 6:J:131:DG:C8    | 2.52                     | 0.44              |
| 6:J:152:DA:C5    | 6:J:153:DG:C5    | 3.06                     | 0.44              |
| 7:U:506:TYR:CE1  | 7:U:520:GLN:HG2  | 2.53                     | 0.44              |
| 7:U:563:MET:SD   | 7:U:589:LEU:HD12 | 2.57                     | 0.44              |
| 7:U:603:LEU:N    | 7:U:631:CYS:O    | 2.51                     | 0.44              |
| 2:L:17:ARG:HD2   | 8:V:533:ILE:HG23 | 2.00                     | 0.44              |
| 8:V:102:LEU:O    | 8:V:106:THR:HG23 | 2.18                     | 0.44              |
| 8:V:800:LYS:HD3  | 8:V:839:LYS:HG3  | 1.98                     | 0.44              |
| 8:V:900:GLY:HA2  | 8:V:947:ILE:HG23 | 2.00                     | 0.44              |
| 8:V:930:PHE:O    | 8:V:934:ILE:N    | 2.50                     | 0.44              |
| 8:V:979:LYS:HD2  | 8:V:981:LYS:HB2  | 1.99                     | 0.44              |
| 8:V:1005:PHE:O   | 8:V:1008:GLY:N   | 2.51                     | 0.44              |
| 1:A:46:VAL:O     | 1:A:50:GLU:OE1   | 2.35                     | 0.44              |
| 4:D:64:ASN:O     | 4:D:67:PHE:N     | 2.50                     | 0.44              |
| 1:E:101:VAL:O    | 1:E:105:GLU:HG2  | 2.18                     | 0.44              |
| 3:G:17:ARG:HH21  | 3:G:28:GLY:HA2   | 1.83                     | 0.44              |
| 5:I:25:DG:H1     | 6:J:290:DC:H42   | 1.66                     | 0.44              |
| 5:I:320:DA:H2'   | 5:I:320:DA:OP2   | 2.18                     | 0.44              |
| 7:U:589:LEU:HD11 | 7:U:720:PHE:CZ   | 2.53                     | 0.44              |
| 8:V:327:HIS:HB3  | 8:V:330:LYS:HZ2  | 1.83                     | 0.44              |
| 3:G:29:ARG:HH21  | 4:H:34:TYR:HD1   | 1.63                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:G:81:ARG:HH12  | 3:G:107:VAL:H     | 1.65                     | 0.43              |
| 5:I:323:DA:C2    | 6:J:-7:DG:C2      | 3.06                     | 0.43              |
| 6:J:60:DA:H2"    | 6:J:61:DA:C8      | 2.53                     | 0.43              |
| 6:J:119:DT:H2"   | 6:J:120:DG:N7     | 2.33                     | 0.43              |
| 7:U:383:LEU:H    | 7:U:388:ARG:CZ    | 2.31                     | 0.43              |
| 2:L:93:GLN:OE1   | 2:L:93:GLN:N      | 2.45                     | 0.43              |
| 1:O:63:ARG:HB3   | 1:O:66:PRO:HD2    | 1.98                     | 0.43              |
| 1:O:99:TYR:N     | 2:P:95:ARG:HH22   | 2.16                     | 0.43              |
| 3:Q:66:ALA:HB1   | 3:Q:78:ILE:HD13   | 2.00                     | 0.43              |
| 8:V:824:TRP:CE2  | 8:V:828:LYS:HB2   | 2.53                     | 0.43              |
| 8:V:996:GLU:O    | 8:V:1000:ILE:HG23 | 2.18                     | 0.43              |
| 8:V:1007:TYR:HE2 | 8:V:1018:VAL:HG12 | 1.83                     | 0.43              |
| 2:F:78:ARG:NE    | 2:F:78:ARG:HA     | 2.33                     | 0.43              |
| 3:G:79:ILE:CD1   | 3:G:81:ARG:HB3    | 2.48                     | 0.43              |
| 7:U:296:SER:HA   | 7:U:376:ASP:OD1   | 2.17                     | 0.43              |
| 2:L:84:MET:O     | 2:L:88:TYR:CD2    | 2.71                     | 0.43              |
| 4:N:53:SER:HA    | 4:N:56:MET:HE3    | 2.00                     | 0.43              |
| 3:Q:83:LEU:HD11  | 4:R:55:ALA:HB1    | 2.00                     | 0.43              |
| 8:V:402:HIS:CG   | 8:V:654:ASN:HA    | 2.52                     | 0.43              |
| 4:D:36:ILE:O     | 4:D:40:LYS:HG3    | 2.18                     | 0.43              |
| 4:D:54:LYS:O     | 4:D:58:ILE:HG13   | 2.18                     | 0.43              |
| 1:K:100:LEU:O    | 1:K:103:LEU:HB3   | 2.17                     | 0.43              |
| 1:K:131:ARG:HH12 | 1:O:131:ARG:CD    | 2.31                     | 0.43              |
| 3:M:41:GLU:HG2   | 3:M:42:ARG:N      | 2.34                     | 0.43              |
| 2:P:26:ILE:HB    | 2:P:59:LYS:HZ3    | 1.84                     | 0.43              |
| 8:V:204:VAL:O    | 8:V:208:VAL:HG13  | 2.18                     | 0.43              |
| 8:V:336:LEU:HA   | 8:V:339:VAL:HG22  | 1.99                     | 0.43              |
| 8:V:886:ASN:HD22 | 8:V:918:LYS:HB2   | 1.82                     | 0.43              |
| 8:V:998:ARG:O    | 8:V:1001:LEU:HG   | 2.18                     | 0.43              |
| 1:A:67:PHE:O     | 1:A:71:VAL:HG23   | 2.18                     | 0.43              |
| 1:A:100:LEU:HB3  | 1:A:104:PHE:CE1   | 2.53                     | 0.43              |
| 3:C:41:GLU:HG2   | 3:C:42:ARG:CG     | 2.47                     | 0.43              |
| 4:H:41:VAL:HA    | 4:H:44:GLN:HB2    | 2.00                     | 0.43              |
| 5:I:158:DG:H2"   | 5:I:159:DA:C8     | 2.52                     | 0.43              |
| 6:J:239:DC:H2"   | 6:J:240:DA:C8     | 2.53                     | 0.43              |
| 7:U:150:VAL:O    | 7:U:430:PRO:HA    | 2.18                     | 0.43              |
| 7:U:210:VAL:HG12 | 7:U:247:ILE:HG23  | 2.00                     | 0.43              |
| 7:U:310:GLY:O    | 7:U:398:TRP:CZ2   | 2.69                     | 0.43              |
| 7:U:339:THR:HB   | 7:U:340:PRO:HD3   | 2.01                     | 0.43              |
| 7:U:452:GLN:CG   | 7:U:509:TRP:HH2   | 2.31                     | 0.43              |
| 7:U:507:ASP:OD1  | 7:U:508:LYS:N     | 2.44                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:U:602:LYS:HG2  | 7:U:632:HIS:HB3   | 1.99                     | 0.43              |
| 1:K:128:ARG:O    | 1:K:132:GLY:N     | 2.51                     | 0.43              |
| 2:L:91:LYS:HE2   | 2:L:92:ARG:HH22   | 1.83                     | 0.43              |
| 3:Q:87:VAL:HG13  | 3:Q:93:LEU:CB     | 2.45                     | 0.43              |
| 8:V:809:LEU:HB3  | 8:V:936:ARG:HH21  | 1.83                     | 0.43              |
| 8:V:1019:ARG:NH1 | 8:V:1023:ARG:HH21 | 2.16                     | 0.43              |
| 3:C:81:ARG:O     | 3:C:85:LEU:HG     | 2.18                     | 0.43              |
| 1:E:101:VAL:HA   | 1:E:104:PHE:HD2   | 1.84                     | 0.43              |
| 2:F:72:TYR:HE2   | 2:F:89:ALA:N      | 2.16                     | 0.43              |
| 4:H:106:HIS:O    | 4:H:109:SER:HB2   | 2.18                     | 0.43              |
| 7:U:225:GLY:C    | 7:U:235:LEU:HD23  | 2.43                     | 0.43              |
| 2:L:98:TYR:CZ    | 4:R:62:PHE:HA     | 2.54                     | 0.43              |
| 4:N:83:ARG:HG2   | 4:N:83:ARG:NH1    | 2.32                     | 0.43              |
| 8:V:258:ASN:ND2  | 8:V:558:ILE:HG23  | 2.34                     | 0.43              |
| 8:V:440:TRP:HA   | 8:V:443:LYS:HB2   | 2.01                     | 0.43              |
| 8:V:564:TYR:CZ   | 8:V:574:PHE:HB2   | 2.53                     | 0.43              |
| 8:V:1031:ASP:OD2 | 8:V:1034:PHE:HD1  | 2.02                     | 0.43              |
| 2:B:30:THR:O     | 2:B:34:ILE:HG13   | 2.19                     | 0.43              |
| 3:C:81:ARG:HH12  | 3:C:107:VAL:N     | 2.16                     | 0.43              |
| 4:D:64:ASN:O     | 4:D:67:PHE:HB3    | 2.18                     | 0.43              |
| 4:D:70:ILE:HG13  | 4:D:71:ALA:N      | 2.33                     | 0.43              |
| 6:J:46:DC:H2''   | 6:J:47:DC:C6      | 2.53                     | 0.43              |
| 6:J:114:DC:H2''  | 6:J:115:DC:H5'    | 2.00                     | 0.43              |
| 1:K:54:TYR:CE1   | 1:K:61:LEU:HD11   | 2.54                     | 0.43              |
| 1:K:78:PHE:CZ    | 2:L:67:ARG:HB2    | 2.53                     | 0.43              |
| 1:O:62:ILE:CD1   | 2:P:33:ALA:HB1    | 2.49                     | 0.43              |
| 2:P:47:SER:OG    | 2:P:48:GLY:N      | 2.51                     | 0.43              |
| 2:P:92:ARG:NH1   | 2:P:92:ARG:O      | 2.51                     | 0.43              |
| 3:Q:81:ARG:O     | 3:Q:85:LEU:HG     | 2.19                     | 0.43              |
| 8:V:184:GLN:HG3  | 8:V:185:PHE:HD2   | 1.84                     | 0.43              |
| 8:V:522:LEU:HD12 | 8:V:593:VAL:HG22  | 1.99                     | 0.43              |
| 8:V:799:PRO:HG3  | 8:V:822:ARG:NH2   | 2.33                     | 0.43              |
| 8:V:942:LYS:O    | 8:V:946:ILE:HG23  | 2.19                     | 0.43              |
| 3:C:18:SER:O     | 3:C:22:GLY:N      | 2.52                     | 0.43              |
| 3:C:90:ASP:OD2   | 3:C:92:GLU:N      | 2.51                     | 0.43              |
| 1:E:65:LEU:O     | 1:E:69:ARG:HG3    | 2.19                     | 0.43              |
| 1:E:85:GLN:CD    | 2:F:82:THR:HA     | 2.44                     | 0.43              |
| 2:F:74:GLU:O     | 2:F:77:LYS:N      | 2.47                     | 0.43              |
| 2:F:94:GLY:O     | 2:F:95:ARG:CZ     | 2.67                     | 0.43              |
| 5:I:129:DT:H1'   | 5:I:130:DC:C4     | 2.54                     | 0.43              |
| 6:J:114:DC:H2'   | 6:J:115:DC:C6     | 2.53                     | 0.43              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 6:J:117:DA:C5    | 6:J:118:DT:C4   | 3.07                     | 0.43              |
| 7:U:265:THR:HG22 | 7:U:266:PHE:CD1 | 2.54                     | 0.43              |
| 2:L:44:LYS:HZ3   | 2:L:45:ARG:HB3  | 1.84                     | 0.43              |
| 4:N:91:ILE:O     | 4:N:95:VAL:HG23 | 2.17                     | 0.43              |
| 8:V:131:PRO:HG2  | 8:V:133:PHE:CD2 | 2.53                     | 0.43              |
| 8:V:820:LYS:O    | 8:V:823:MET:HB3 | 2.18                     | 0.43              |
| 8:V:1005:PHE:CA  | 8:V:1008:GLY:H  | 2.32                     | 0.43              |
| 2:B:33:ALA:O     | 2:B:37:LEU:HD23 | 2.19                     | 0.43              |
| 1:E:83:ARG:HG2   | 5:I:51:DC:H5'   | 2.00                     | 0.43              |
| 7:U:536:GLN:O    | 7:U:536:GLN:HG2 | 2.19                     | 0.43              |
| 1:K:122:LYS:O    | 1:K:126:LEU:HB2 | 2.19                     | 0.43              |
| 4:N:62:PHE:HD1   | 2:P:98:TYR:CE2  | 2.36                     | 0.43              |
| 1:O:84:PHE:HA    | 2:P:81:VAL:HB   | 2.01                     | 0.43              |
| 1:A:89:VAL:HA    | 1:A:92:LEU:HD12 | 2.01                     | 0.43              |
| 1:A:93:GLN:O     | 1:A:94:GLU:C    | 2.58                     | 0.43              |
| 1:E:75:ALA:HB2   | 2:F:66:ILE:HD11 | 2.00                     | 0.43              |
| 2:F:72:TYR:CE2   | 2:F:88:TYR:HB2  | 2.53                     | 0.43              |
| 6:J:102:DA:H2''  | 6:J:103:DG:C8   | 2.53                     | 0.43              |
| 7:U:154:LEU:C    | 7:U:156:SER:H   | 2.25                     | 0.43              |
| 7:U:181:ASP:OD2  | 7:U:393:ARG:NE  | 2.51                     | 0.43              |
| 7:U:650:LYS:HA   | 7:U:700:ARG:CD  | 2.49                     | 0.43              |
| 2:L:63:GLU:O     | 2:L:66:ILE:N    | 2.52                     | 0.43              |
| 4:R:81:ASN:OD1   | 4:R:81:ASN:C    | 2.60                     | 0.43              |
| 3:C:74:LYS:HD3   | 3:C:74:LYS:N    | 2.34                     | 0.43              |
| 4:H:33:SER:OG    | 4:H:60:ASN:OD1  | 2.25                     | 0.43              |
| 5:I:105:DT:H3    | 6:J:210:DA:H61  | 1.65                     | 0.43              |
| 5:I:322:DC:OP2   | 5:I:322:DC:H6   | 2.02                     | 0.43              |
| 5:I:337:DT:H2''  | 5:I:338:DT:C6   | 2.54                     | 0.43              |
| 6:J:2:DC:H2''    | 6:J:3:DA:H5''   | 2.01                     | 0.43              |
| 7:U:646:TYR:O    | 7:U:649:VAL:HB  | 2.18                     | 0.43              |
| 7:U:706:LEU:HD13 | 7:U:706:LEU:HA  | 1.91                     | 0.43              |
| 3:M:28:GLY:O     | 3:M:32:ARG:HD3  | 2.18                     | 0.43              |
| 3:M:83:LEU:HD13  | 4:N:58:ILE:HG21 | 2.01                     | 0.43              |
| 4:R:86:ILE:O     | 4:R:86:ILE:HG13 | 2.19                     | 0.43              |
| 8:V:413:ILE:HG22 | 8:V:415:SER:H   | 1.84                     | 0.43              |
| 4:H:74:ALA:HA    | 4:H:77:LEU:HG   | 2.00                     | 0.42              |
| 4:H:109:SER:HB3  | 4:H:113:LYS:NZ  | 2.33                     | 0.42              |
| 6:J:-2:DC:C2     | 6:J:-1:DG:C5    | 3.06                     | 0.42              |
| 7:U:197:HIS:O    | 7:U:200:LEU:HB2 | 2.19                     | 0.42              |
| 7:U:394:ALA:O    | 7:U:398:TRP:CE3 | 2.72                     | 0.42              |
| 1:K:54:TYR:HA    | 1:K:57:SER:OG   | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:101:VAL:O    | 1:O:104:PHE:HB2  | 2.19                     | 0.42              |
| 3:Q:63:LEU:HD23  | 3:Q:63:LEU:HA    | 1.87                     | 0.42              |
| 3:C:47:ALA:HB3   | 3:C:48:PRO:HD3   | 2.00                     | 0.42              |
| 4:D:88:SER:O     | 4:D:91:ILE:HG22  | 2.19                     | 0.42              |
| 2:F:82:THR:O     | 2:F:85:ASP:HB2   | 2.19                     | 0.42              |
| 3:G:90:ASP:HB3   | 3:G:93:LEU:HB2   | 2.00                     | 0.42              |
| 5:I:132:DG:C4    | 5:I:133:DA:C5    | 3.07                     | 0.42              |
| 5:I:158:DG:H2"   | 5:I:159:DA:H8    | 1.83                     | 0.42              |
| 5:I:287:DA:N1    | 6:J:27:DC:C2     | 2.87                     | 0.42              |
| 6:J:129:DC:H2"   | 6:J:130:DG:N7    | 2.34                     | 0.42              |
| 7:U:136:GLU:O    | 7:U:457:ILE:HD12 | 2.19                     | 0.42              |
| 7:U:228:LYS:H    | 7:U:232:ASP:CB   | 2.31                     | 0.42              |
| 7:U:333:PHE:O    | 7:U:335:GLN:NE2  | 2.52                     | 0.42              |
| 7:U:444:PHE:HD2  | 7:U:502:LEU:HD21 | 1.84                     | 0.42              |
| 3:M:30:VAL:HG12  | 3:M:34:LEU:HG    | 2.01                     | 0.42              |
| 3:M:30:VAL:O     | 3:M:34:LEU:HG    | 2.19                     | 0.42              |
| 3:M:43:VAL:HG12  | 3:M:44:GLY:O     | 2.19                     | 0.42              |
| 2:P:52:GLU:OE1   | 2:P:55:ARG:NH1   | 2.50                     | 0.42              |
| 8:V:823:MET:HG3  | 8:V:864:ASN:CG   | 2.44                     | 0.42              |
| 8:V:905:ASN:O    | 8:V:907:ILE:HG13 | 2.18                     | 0.42              |
| 2:B:47:SER:HB3   | 2:B:50:ILE:HG12  | 2.00                     | 0.42              |
| 1:E:52:ARG:C     | 1:E:56:LYS:HZ2   | 2.26                     | 0.42              |
| 3:G:29:ARG:O     | 3:G:33:LEU:HG    | 2.19                     | 0.42              |
| 4:H:65:ASP:C     | 4:H:65:ASP:OD1   | 2.63                     | 0.42              |
| 1:K:94:GLU:O     | 1:K:97:GLU:HG3   | 2.19                     | 0.42              |
| 1:K:120:MET:HB2  | 1:K:122:LYS:HG2  | 2.00                     | 0.42              |
| 3:M:52:ALA:O     | 3:M:55:LEU:N     | 2.52                     | 0.42              |
| 3:M:83:LEU:HA    | 3:M:83:LEU:HD23  | 1.82                     | 0.42              |
| 2:P:71:THR:O     | 2:P:74:GLU:HG3   | 2.18                     | 0.42              |
| 3:Q:17:ARG:HH21  | 3:Q:28:GLY:HA2   | 1.82                     | 0.42              |
| 3:Q:34:LEU:HD12  | 3:Q:48:PRO:HG3   | 2.00                     | 0.42              |
| 4:R:36:ILE:HD11  | 4:R:37:TYR:CZ    | 2.54                     | 0.42              |
| 4:R:77:LEU:HD23  | 4:R:77:LEU:HA    | 1.89                     | 0.42              |
| 8:V:285:GLU:O    | 8:V:289:LYS:HB3  | 2.19                     | 0.42              |
| 8:V:356:LEU:HD22 | 8:V:363:LEU:HB2  | 2.01                     | 0.42              |
| 8:V:769:ARG:HG2  | 8:V:771:ARG:HG3  | 2.01                     | 0.42              |
| 8:V:799:PRO:HG2  | 8:V:837:ASP:O    | 2.18                     | 0.42              |
| 8:V:855:LEU:HD11 | 8:V:859:LYS:HE3  | 2.01                     | 0.42              |
| 1:A:95:ALA:HB2   | 2:B:90:LEU:HD22  | 2.01                     | 0.42              |
| 2:B:46:ILE:HG22  | 2:B:47:SER:O     | 2.20                     | 0.42              |
| 4:D:43:LYS:HA    | 4:D:47:PRO:HA    | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:U:154:LEU:O    | 7:U:156:SER:N    | 2.48                     | 0.42              |
| 7:U:168:LEU:HD11 | 7:U:605:TYR:CD2  | 2.54                     | 0.42              |
| 7:U:176:VAL:HG21 | 7:U:604:PHE:CE1  | 2.55                     | 0.42              |
| 7:U:417:LYS:HD2  | 7:U:417:LYS:N    | 2.35                     | 0.42              |
| 1:K:121:PRO:O    | 1:K:124:ILE:N    | 2.53                     | 0.42              |
| 8:V:367:LEU:HD11 | 8:V:375:PHE:CZ   | 2.54                     | 0.42              |
| 8:V:434:SER:N    | 8:V:502:ALA:HB2  | 2.35                     | 0.42              |
| 4:D:106:HIS:CE1  | 7:U:739:ARG:HE   | 2.36                     | 0.42              |
| 5:I:303:DT:H2''  | 5:I:304:DA:C8    | 2.54                     | 0.42              |
| 6:J:39:DG:H4'    | 3:M:42:ARG:HH11  | 1.85                     | 0.42              |
| 7:U:170:ASN:ND2  | 7:U:172:ASN:HB2  | 2.33                     | 0.42              |
| 7:U:603:LEU:O    | 7:U:630:LEU:N    | 2.35                     | 0.42              |
| 7:U:736:GLN:O    | 7:U:739:ARG:HB2  | 2.18                     | 0.42              |
| 2:P:78:ARG:NH1   | 2:P:82:THR:HG23  | 2.35                     | 0.42              |
| 8:V:310:LYS:O    | 8:V:314:LYS:HG3  | 2.19                     | 0.42              |
| 8:V:570:LYS:O    | 8:V:572:PHE:N    | 2.52                     | 0.42              |
| 8:V:823:MET:HE3  | 8:V:861:SER:HA   | 2.01                     | 0.42              |
| 8:V:824:TRP:HE3  | 8:V:867:PRO:HB3  | 1.84                     | 0.42              |
| 8:V:868:LEU:HA   | 8:V:872:GLU:OE1  | 2.19                     | 0.42              |
| 3:G:79:ILE:HD11  | 3:G:81:ARG:HB3   | 2.02                     | 0.42              |
| 4:H:93:THR:O     | 4:H:96:ARG:HB2   | 2.19                     | 0.42              |
| 5:I:183:DG:C2    | 6:J:133:DA:C2    | 3.07                     | 0.42              |
| 6:J:103:DG:C2    | 6:J:104:DC:C2    | 3.08                     | 0.42              |
| 7:U:247:ILE:O    | 7:U:251:GLN:HG3  | 2.19                     | 0.42              |
| 7:U:478:ARG:HA   | 7:U:481:GLU:HG2  | 2.02                     | 0.42              |
| 3:Q:77:ARG:HG2   | 4:R:50:GLY:CA    | 2.45                     | 0.42              |
| 8:V:808:GLN:HB3  | 8:V:884:PHE:O    | 2.19                     | 0.42              |
| 8:V:887:TRP:HZ2  | 8:V:922:GLU:HG3  | 1.84                     | 0.42              |
| 3:C:27:VAL:HA    | 3:C:30:VAL:HG12  | 2.02                     | 0.42              |
| 5:I:156:DG:H2''  | 5:I:157:DA:C8    | 2.54                     | 0.42              |
| 6:J:146:DA:C6    | 6:J:147:DG:C5    | 3.08                     | 0.42              |
| 7:U:526:PHE:CZ   | 7:U:566:PHE:HB3  | 2.55                     | 0.42              |
| 7:U:641:LEU:HA   | 7:U:644:LEU:HG   | 2.01                     | 0.42              |
| 2:L:31:LYS:HE2   | 2:L:51:TYR:OH    | 2.20                     | 0.42              |
| 3:M:78:ILE:N     | 4:N:50:GLY:O     | 2.48                     | 0.42              |
| 1:O:108:ASN:O    | 1:O:112:ILE:HG12 | 2.20                     | 0.42              |
| 8:V:222:GLU:OE1  | 8:V:414:LYS:HB2  | 2.19                     | 0.42              |
| 8:V:898:VAL:HA   | 8:V:901:LYS:HD3  | 2.00                     | 0.42              |
| 3:C:96:LEU:HD12  | 3:C:96:LEU:HA    | 1.85                     | 0.42              |
| 5:I:89:DT:H4'    | 5:I:90:DA:OP1    | 2.20                     | 0.42              |
| 6:J:120:DG:H1'   | 6:J:121:DA:C8    | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:J:135:DC:H6    | 6:J:135:DC:H2'   | 1.64                     | 0.42              |
| 6:J:152:DA:C4    | 6:J:153:DG:C5    | 3.07                     | 0.42              |
| 7:U:159:LYS:HA   | 7:U:161:GLN:NE2  | 2.34                     | 0.42              |
| 7:U:336:ASP:N    | 7:U:336:ASP:OD1  | 2.52                     | 0.42              |
| 7:U:350:LEU:HD13 | 8:V:903:GLY:HA3  | 2.02                     | 0.42              |
| 7:U:400:ALA:O    | 8:V:1036:SER:OG  | 2.30                     | 0.42              |
| 7:U:643:PHE:CE1  | 7:U:686:ASN:HB2  | 2.54                     | 0.42              |
| 1:K:130:ILE:O    | 1:O:131:ARG:NH2  | 2.52                     | 0.42              |
| 2:L:59:LYS:HA    | 2:L:62:LEU:HD12  | 2.02                     | 0.42              |
| 1:O:83:ARG:HB3   | 2:P:80:THR:HA    | 2.01                     | 0.42              |
| 1:O:116:ARG:HH22 | 1:O:123:ASP:CG   | 2.27                     | 0.42              |
| 8:V:113:LEU:O    | 8:V:120:LYS:NZ   | 2.50                     | 0.42              |
| 8:V:199:TYR:CE2  | 8:V:225:LEU:HB3  | 2.55                     | 0.42              |
| 8:V:361:HIS:HA   | 8:V:364:TRP:HE1  | 1.84                     | 0.42              |
| 8:V:797:ARG:HD3  | 8:V:831:TYR:CD2  | 2.55                     | 0.42              |
| 8:V:808:GLN:HB3  | 8:V:884:PHE:C    | 2.45                     | 0.42              |
| 8:V:884:PHE:HB3  | 8:V:887:TRP:CD1  | 2.54                     | 0.42              |
| 8:V:917:GLY:O    | 8:V:918:LYS:HE2  | 2.20                     | 0.42              |
| 2:B:72:TYR:CE2   | 2:B:88:TYR:HB3   | 2.55                     | 0.42              |
| 3:C:99:ARG:O     | 2:F:96:THR:OG1   | 2.26                     | 0.42              |
| 3:G:15:LYS:HB2   | 3:G:20:ARG:CZ    | 2.50                     | 0.42              |
| 3:G:51:LEU:O     | 3:G:55:LEU:HG    | 2.20                     | 0.42              |
| 3:G:94:ASN:O     | 3:G:98:GLY:N     | 2.53                     | 0.42              |
| 4:H:37:TYR:O     | 4:H:41:VAL:HG22  | 2.20                     | 0.42              |
| 5:I:163:DT:C2    | 5:I:164:DC:C4    | 3.07                     | 0.42              |
| 6:J:9:DT:H2''    | 6:J:10:DA:C8     | 2.55                     | 0.42              |
| 6:J:47:DC:H1'    | 6:J:48:DC:C6     | 2.55                     | 0.42              |
| 2:L:26:ILE:HG23  | 2:L:27:GLN:OE1   | 2.20                     | 0.42              |
| 2:L:63:GLU:HG2   | 2:L:64:ASN:N     | 2.34                     | 0.42              |
| 8:V:258:ASN:ND2  | 8:V:558:ILE:HG12 | 2.35                     | 0.42              |
| 8:V:274:PHE:CZ   | 8:V:290:LYS:HD3  | 2.55                     | 0.42              |
| 8:V:306:ILE:HG13 | 8:V:307:ILE:N    | 2.35                     | 0.42              |
| 8:V:359:ASN:O    | 8:V:362:GLU:HB3  | 2.19                     | 0.42              |
| 8:V:436:MET:HG2  | 8:V:500:ASN:HD22 | 1.84                     | 0.42              |
| 8:V:577:THR:OG1  | 8:V:580:ALA:HB3  | 2.20                     | 0.42              |
| 8:V:968:LEU:HD13 | 8:V:1005:PHE:HB3 | 2.02                     | 0.42              |
| 2:B:50:ILE:O     | 2:B:53:GLU:HB3   | 2.20                     | 0.42              |
| 3:G:39:TYR:OH    | 4:H:68:GLU:OE1   | 2.37                     | 0.42              |
| 5:I:317:DG:C4    | 5:I:318:DT:C4    | 3.08                     | 0.42              |
| 6:J:-11:DC:H2''  | 6:J:-10:DC:C5    | 2.55                     | 0.42              |
| 6:J:57:DT:H2'    | 6:J:58:DT:H72    | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:J:57:DT:H4'     | 8:V:308:ARG:NH1   | 2.35                     | 0.42              |
| 6:J:178:DT:H2'    | 6:J:179:DA:C8     | 2.54                     | 0.42              |
| 7:U:437:VAL:HG13  | 7:U:438:ASP:OD1   | 2.20                     | 0.42              |
| 7:U:551:MET:HE1   | 7:U:601:PHE:CD2   | 2.55                     | 0.42              |
| 3:M:26:PRO:HG3    | 4:N:37:TYR:CE2    | 2.55                     | 0.42              |
| 8:V:425:LYS:N     | 8:V:621:VAL:O     | 2.44                     | 0.42              |
| 3:G:97:LEU:HD21   | 4:H:62:PHE:CZ     | 2.55                     | 0.41              |
| 4:H:58:ILE:HG22   | 4:H:59:MET:HE2    | 2.02                     | 0.41              |
| 5:I:19:DG:H2''    | 5:I:20:DA:C8      | 2.55                     | 0.41              |
| 6:J:43:DA:C6      | 6:J:44:DA:C6      | 3.08                     | 0.41              |
| 7:U:161:GLN:OE1   | 7:U:161:GLN:N     | 2.53                     | 0.41              |
| 7:U:634:SER:O     | 7:U:637:LEU:HB3   | 2.19                     | 0.41              |
| 1:K:60:LEU:HD13   | 1:K:62:ILE:O      | 2.20                     | 0.41              |
| 2:L:84:MET:HE2    | 2:L:88:TYR:CE2    | 2.55                     | 0.41              |
| 2:P:61:PHE:O      | 2:P:65:VAL:HG23   | 2.20                     | 0.41              |
| 8:V:304:GLU:O     | 8:V:308:ARG:HG2   | 2.20                     | 0.41              |
| 8:V:332:GLU:O     | 8:V:337:SER:OG    | 2.27                     | 0.41              |
| 8:V:820:LYS:HA    | 8:V:823:MET:HB2   | 2.02                     | 0.41              |
| 8:V:956:ARG:HA    | 8:V:959:MET:SD    | 2.59                     | 0.41              |
| 8:V:997:ASP:HA    | 8:V:1000:ILE:HG12 | 2.01                     | 0.41              |
| 3:C:74:LYS:C      | 3:C:75:LYS:HD3    | 2.45                     | 0.41              |
| 3:G:81:ARG:CZ     | 3:G:85:LEU:HD21   | 2.50                     | 0.41              |
| 5:I:219:DA:C6     | 6:J:97:DG:C6      | 3.08                     | 0.41              |
| 6:J:41:DG:H2''    | 6:J:42:DT:O5'     | 2.20                     | 0.41              |
| 6:J:159:DC:H4'    | 6:J:160:DG:H5'    | 2.02                     | 0.41              |
| 7:U:262:LEU:HA    | 7:U:262:LEU:HD23  | 1.76                     | 0.41              |
| 7:U:560:SER:O     | 7:U:564:SER:HB2   | 2.19                     | 0.41              |
| 7:U:702:LYS:O     | 7:U:706:LEU:HD23  | 2.20                     | 0.41              |
| 2:L:58:LEU:HA     | 2:L:58:LEU:HD13   | 1.81                     | 0.41              |
| 2:P:92:ARG:HH11   | 2:P:92:ARG:HA     | 1.85                     | 0.41              |
| 3:Q:102:ILE:CG2   | 3:Q:105:GLY:HA3   | 2.50                     | 0.41              |
| 4:R:73:GLU:HA     | 4:R:73:GLU:OE2    | 2.21                     | 0.41              |
| 8:V:118:LEU:HD22  | 8:V:404:VAL:HG21  | 2.02                     | 0.41              |
| 8:V:866:GLN:N     | 8:V:867:PRO:HD3   | 2.35                     | 0.41              |
| 8:V:896:ILE:HD12  | 8:V:930:PHE:HZ    | 1.84                     | 0.41              |
| 8:V:1058:ASN:HD22 | 8:V:1058:ASN:HA   | 1.65                     | 0.41              |
| 1:A:65:LEU:O      | 1:A:69:ARG:HG3    | 2.18                     | 0.41              |
| 1:E:97:GLU:HA     | 1:E:100:LEU:HD21  | 2.02                     | 0.41              |
| 1:E:121:PRO:HA    | 1:E:124:ILE:HG22  | 2.01                     | 0.41              |
| 7:U:257:LEU:HD12  | 7:U:258:PHE:N     | 2.35                     | 0.41              |
| 7:U:555:HIS:HE1   | 7:U:557:TYR:HB2   | 1.78                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:U:682:ASN:C     | 7:U:684:SER:H     | 2.28                     | 0.41              |
| 2:L:20:LYS:C      | 2:L:20:LYS:HD2    | 2.44                     | 0.41              |
| 4:N:34:TYR:O      | 4:N:38:VAL:HG23   | 2.21                     | 0.41              |
| 1:O:100:LEU:HD23  | 1:O:100:LEU:HA    | 1.85                     | 0.41              |
| 4:R:41:VAL:O      | 4:R:44:GLN:HB2    | 2.20                     | 0.41              |
| 8:V:191:TYR:CE2   | 8:V:236:GLY:HA3   | 2.54                     | 0.41              |
| 2:B:74:GLU:O      | 2:B:77:LYS:N      | 2.37                     | 0.41              |
| 5:I:182:DT:H2''   | 5:I:183:DG:H8     | 1.83                     | 0.41              |
| 5:I:287:DA:C2     | 5:I:288:DG:C2     | 3.08                     | 0.41              |
| 7:U:139:GLU:HB3   | 7:U:454:ARG:HG3   | 2.01                     | 0.41              |
| 7:U:327:LYS:HZ2   | 8:V:1006:LYS:C    | 2.28                     | 0.41              |
| 7:U:334:GLU:HB2   | 7:U:354:ILE:N     | 2.35                     | 0.41              |
| 3:M:62:ILE:O      | 3:M:65:LEU:HB2    | 2.21                     | 0.41              |
| 4:N:33:SER:HB2    | 4:N:60:ASN:ND2    | 2.35                     | 0.41              |
| 1:O:133:GLU:OE1   | 1:O:133:GLU:N     | 2.46                     | 0.41              |
| 8:V:199:TYR:HE2   | 8:V:225:LEU:HB3   | 1.86                     | 0.41              |
| 8:V:434:SER:HB3   | 8:V:437:GLN:HG2   | 2.02                     | 0.41              |
| 8:V:959:MET:HB3   | 8:V:1065:ASP:OD1  | 2.20                     | 0.41              |
| 8:V:1001:LEU:HD12 | 8:V:1002:LEU:N    | 2.35                     | 0.41              |
| 1:A:54:TYR:HB3    | 2:B:40:ARG:HB2    | 2.02                     | 0.41              |
| 3:C:71:ARG:HH11   | 3:C:71:ARG:HG3    | 1.86                     | 0.41              |
| 2:F:60:VAL:HA     | 2:F:63:GLU:OE2    | 2.21                     | 0.41              |
| 3:G:65:LEU:HD23   | 3:G:65:LEU:HA     | 1.90                     | 0.41              |
| 5:I:311:DC:C2     | 6:J:5:DG:N2       | 2.88                     | 0.41              |
| 6:J:145:DC:H4'    | 6:J:146:DA:OP1    | 2.20                     | 0.41              |
| 6:J:158:DT:H2''   | 6:J:159:DC:H5'    | 2.01                     | 0.41              |
| 7:U:267:THR:CB    | 7:U:281:LEU:HD21  | 2.50                     | 0.41              |
| 1:E:118:THR:HA    | 2:F:45:ARG:O      | 2.20                     | 0.41              |
| 5:I:288:DG:H2''   | 5:I:289:DG:C8     | 2.56                     | 0.41              |
| 7:U:546:ILE:HG22  | 7:U:605:TYR:CE1   | 2.56                     | 0.41              |
| 1:K:131:ARG:NH1   | 1:O:131:ARG:HA    | 2.36                     | 0.41              |
| 3:M:29:ARG:NH1    | 4:N:33:SER:O      | 2.31                     | 0.41              |
| 4:R:99:LEU:HB2    | 4:R:104:ALA:HB2   | 2.03                     | 0.41              |
| 8:V:1007:TYR:CD2  | 8:V:1014:VAL:HG13 | 2.56                     | 0.41              |
| 3:G:44:GLY:N      | 4:H:86:ILE:O      | 2.40                     | 0.41              |
| 7:U:163:SER:HB3   | 7:U:545:HIS:HA    | 2.01                     | 0.41              |
| 7:U:341:VAL:HA    | 8:V:907:ILE:HD11  | 2.03                     | 0.41              |
| 7:U:342:VAL:HB    | 8:V:924:ARG:HG3   | 2.02                     | 0.41              |
| 7:U:431:ARG:O     | 7:U:434:ILE:HG22  | 2.21                     | 0.41              |
| 7:U:509:TRP:CE3   | 7:U:512:LEU:HD12  | 2.56                     | 0.41              |
| 1:K:83:ARG:O      | 2:L:80:THR:HG23   | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:87:SER:HA    | 1:K:90:MET:CE    | 2.49                     | 0.41              |
| 1:A:108:ASN:O    | 1:A:112:ILE:HG12 | 2.20                     | 0.41              |
| 1:E:100:LEU:HD12 | 1:E:101:VAL:N    | 2.36                     | 0.41              |
| 5:I:217:DG:C2    | 6:J:99:DT:O2     | 2.73                     | 0.41              |
| 6:J:-25:DG:H2''  | 6:J:-24:DG:C8    | 2.55                     | 0.41              |
| 6:J:-6:DA:H2''   | 6:J:-5:DT:H71    | 2.03                     | 0.41              |
| 6:J:144:DC:H5''  | 1:K:42:ARG:HG2   | 2.01                     | 0.41              |
| 6:J:151:DG:H4'   | 6:J:152:DA:H5'   | 2.03                     | 0.41              |
| 7:U:218:ASP:CG   | 7:U:220:ASN:H    | 2.29                     | 0.41              |
| 7:U:283:THR:H    | 7:U:286:ASN:HB3  | 1.85                     | 0.41              |
| 7:U:383:LEU:HD23 | 7:U:387:ASP:HB3  | 2.02                     | 0.41              |
| 2:L:92:ARG:NH1   | 4:N:76:ARG:HH12  | 2.18                     | 0.41              |
| 8:V:197:ARG:NH2  | 8:V:419:THR:HG22 | 2.35                     | 0.41              |
| 8:V:252:ALA:HB1  | 8:V:256:THR:OG1  | 2.21                     | 0.41              |
| 8:V:286:LEU:HD23 | 8:V:286:LEU:HA   | 1.83                     | 0.41              |
| 8:V:480:TYR:HD1  | 8:V:486:GLU:HB2  | 1.83                     | 0.41              |
| 8:V:520:ARG:HH22 | 8:V:569:SER:CB   | 2.34                     | 0.41              |
| 8:V:921:GLU:OE1  | 8:V:924:ARG:HD3  | 2.21                     | 0.41              |
| 3:C:85:LEU:HD23  | 3:C:108:LEU:HD23 | 2.03                     | 0.41              |
| 2:F:63:GLU:HG2   | 2:F:64:ASN:N     | 2.36                     | 0.41              |
| 3:G:97:LEU:CD1   | 3:G:100:VAL:HG21 | 2.51                     | 0.41              |
| 5:I:90:DA:H1'    | 5:I:91:DA:N7     | 2.36                     | 0.41              |
| 5:I:131:DA:C5    | 5:I:132:DG:C6    | 3.09                     | 0.41              |
| 5:I:164:DC:C2    | 5:I:165:DG:N7    | 2.89                     | 0.41              |
| 5:I:181:DG:C2'   | 5:I:182:DT:H71   | 2.51                     | 0.41              |
| 6:J:-10:DC:H2''  | 6:J:-9:DA:H8     | 1.85                     | 0.41              |
| 6:J:93:DC:H2''   | 6:J:94:DG:C8     | 2.56                     | 0.41              |
| 7:U:181:ASP:O    | 7:U:185:LEU:HG   | 2.20                     | 0.41              |
| 7:U:291:SER:C    | 7:U:293:LYS:H    | 2.29                     | 0.41              |
| 7:U:299:LEU:HD21 | 7:U:303:ARG:HH22 | 1.86                     | 0.41              |
| 7:U:383:LEU:HB2  | 7:U:388:ARG:HG3  | 2.02                     | 0.41              |
| 2:L:68:ASP:O     | 2:L:71:THR:HB    | 2.20                     | 0.41              |
| 3:M:67:GLY:HA3   | 4:N:46:HIS:CD2   | 2.56                     | 0.41              |
| 4:N:105:LYS:HB3  | 8:V:765:ASN:OD1  | 2.21                     | 0.41              |
| 1:O:67:PHE:O     | 1:O:71:VAL:HG23  | 2.21                     | 0.41              |
| 1:O:85:GLN:NE2   | 2:P:82:THR:HG22  | 2.36                     | 0.41              |
| 8:V:121:HIS:CE1  | 8:V:384:TRP:HE1  | 2.38                     | 0.41              |
| 8:V:239:ARG:NH2  | 8:V:270:ASP:HB3  | 2.35                     | 0.41              |
| 8:V:405:LEU:O    | 8:V:409:LEU:N    | 2.54                     | 0.41              |
| 8:V:520:ARG:NH1  | 8:V:569:SER:O    | 2.54                     | 0.41              |
| 8:V:647:ASP:O    | 8:V:651:ILE:HG12 | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:V:934:ILE:HG13 | 8:V:940:TYR:CD2  | 2.55                     | 0.41              |
| 8:V:953:LYS:O    | 8:V:956:ARG:HB3  | 2.21                     | 0.41              |
| 3:C:25:PHE:HE2   | 3:C:55:LEU:HB3   | 1.86                     | 0.41              |
| 3:G:62:ILE:HD13  | 3:G:93:LEU:HD13  | 2.02                     | 0.41              |
| 5:I:330:DT:H2''  | 5:I:331:DA:C8    | 2.56                     | 0.41              |
| 6:J:-21:DA:H2''  | 6:J:-20:DC:C6    | 2.56                     | 0.41              |
| 6:J:56:DG:C8     | 6:J:57:DT:H72    | 2.56                     | 0.41              |
| 7:U:456:GLU:OE2  | 7:U:487:LYS:HG3  | 2.21                     | 0.41              |
| 8:V:1019:ARG:HB2 | 8:V:1039:PRO:HG3 | 2.03                     | 0.41              |
| 2:B:77:LYS:HZ3   | 4:D:89:ARG:NH2   | 2.19                     | 0.40              |
| 3:C:18:SER:HA    | 3:C:23:LEU:HB3   | 2.03                     | 0.40              |
| 3:C:97:LEU:HD11  | 4:D:62:PHE:HE1   | 1.86                     | 0.40              |
| 4:D:41:VAL:O     | 4:D:44:GLN:HB2   | 2.21                     | 0.40              |
| 1:E:109:LEU:HA   | 1:E:112:ILE:HG12 | 2.01                     | 0.40              |
| 5:I:164:DC:O2    | 6:J:152:DA:C2    | 2.73                     | 0.40              |
| 5:I:287:DA:H1'   | 5:I:288:DG:C5    | 2.56                     | 0.40              |
| 6:J:184:DT:H2''  | 6:J:185:DG:N7    | 2.36                     | 0.40              |
| 6:J:237:DG:H2''  | 6:J:238:DA:C8    | 2.56                     | 0.40              |
| 7:U:444:PHE:CE1  | 7:U:447:LEU:HD22 | 2.57                     | 0.40              |
| 7:U:466:LYS:HE3  | 7:U:466:LYS:HB2  | 1.93                     | 0.40              |
| 7:U:590:PHE:HA   | 7:U:594:GLY:CA   | 2.47                     | 0.40              |
| 1:K:128:ARG:O    | 1:K:133:GLU:N    | 2.51                     | 0.40              |
| 2:L:44:LYS:HZ3   | 2:L:45:ARG:CB    | 2.34                     | 0.40              |
| 1:O:122:LYS:O    | 1:O:126:LEU:HD23 | 2.21                     | 0.40              |
| 8:V:835:MET:SD   | 8:V:854:LYS:HD2  | 2.61                     | 0.40              |
| 8:V:1005:PHE:C   | 8:V:1008:GLY:N   | 2.77                     | 0.40              |
| 3:G:18:SER:HB2   | 3:G:23:LEU:HB3   | 2.04                     | 0.40              |
| 4:H:53:SER:O     | 4:H:56:MET:HB3   | 2.21                     | 0.40              |
| 4:H:99:LEU:HA    | 4:H:100:PRO:HD3  | 1.74                     | 0.40              |
| 6:J:-22:DA:H2''  | 6:J:-21:DA:C8    | 2.55                     | 0.40              |
| 6:J:-19:DA:H2''  | 6:J:-18:DG:C8    | 2.56                     | 0.40              |
| 6:J:3:DA:C6      | 6:J:4:DG:C6      | 3.09                     | 0.40              |
| 6:J:146:DA:C6    | 6:J:147:DG:C6    | 3.10                     | 0.40              |
| 7:U:338:GLN:NE2  | 8:V:909:ALA:H    | 2.18                     | 0.40              |
| 7:U:478:ARG:HE   | 7:U:481:GLU:CD   | 2.28                     | 0.40              |
| 7:U:538:PHE:CD1  | 7:U:552:PRO:HA   | 2.56                     | 0.40              |
| 7:U:567:THR:HG23 | 7:U:572:LEU:HB2  | 2.03                     | 0.40              |
| 7:U:601:PHE:O    | 7:U:602:LYS:HG3  | 2.21                     | 0.40              |
| 3:M:42:ARG:HB2   | 4:N:85:THR:OG1   | 2.21                     | 0.40              |
| 1:O:48:LEU:CD1   | 2:P:44:LYS:HE3   | 2.51                     | 0.40              |
| 2:P:84:MET:HG2   | 2:P:88:TYR:CE2   | 2.57                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:V:109:PHE:CD1  | 8:V:112:LEU:HD12 | 2.56                     | 0.40              |
| 8:V:120:LYS:H    | 8:V:120:LYS:CD   | 2.34                     | 0.40              |
| 8:V:281:GLU:HG2  | 8:V:282:GLU:N    | 2.36                     | 0.40              |
| 8:V:432:GLY:HA2  | 8:V:629:ASP:HB3  | 2.03                     | 0.40              |
| 8:V:532:ASP:HA   | 8:V:547:ARG:NH1  | 2.36                     | 0.40              |
| 8:V:854:LYS:NZ   | 8:V:858:LEU:HD12 | 2.36                     | 0.40              |
| 8:V:908:GLN:HB3  | 8:V:912:ARG:NH1  | 2.35                     | 0.40              |
| 3:C:99:ARG:HA    | 3:C:99:ARG:NE    | 2.36                     | 0.40              |
| 3:G:70:ALA:HA    | 3:G:82:HIS:CD2   | 2.56                     | 0.40              |
| 6:J:81:DC:H2''   | 6:J:82:DG:C8     | 2.57                     | 0.40              |
| 6:J:158:DT:H2''  | 6:J:159:DC:H2'   | 2.03                     | 0.40              |
| 7:U:249:TYR:O    | 7:U:253:LYS:HG2  | 2.21                     | 0.40              |
| 7:U:284:TRP:HB3  | 7:U:288:LYS:NZ   | 2.35                     | 0.40              |
| 7:U:410:ILE:HG13 | 7:U:411:TYR:N    | 2.36                     | 0.40              |
| 7:U:555:HIS:HD2  | 7:U:560:SER:HB2  | 1.86                     | 0.40              |
| 7:U:700:ARG:HA   | 7:U:703:LEU:HB2  | 2.02                     | 0.40              |
| 1:K:129:ARG:C    | 1:K:132:GLY:H    | 2.29                     | 0.40              |
| 2:L:83:ALA:O     | 2:L:86:VAL:HG12  | 2.20                     | 0.40              |
| 3:M:50:TYR:CD1   | 4:N:88:SER:HB2   | 2.56                     | 0.40              |
| 3:M:77:ARG:HG2   | 4:N:50:GLY:HA3   | 2.02                     | 0.40              |
| 4:R:73:GLU:HG2   | 4:R:98:LEU:HD11  | 2.03                     | 0.40              |
| 8:V:908:GLN:HB3  | 8:V:912:ARG:CZ   | 2.52                     | 0.40              |
| 3:C:98:GLY:O     | 3:C:99:ARG:NH2   | 2.55                     | 0.40              |
| 4:D:52:SER:HB3   | 4:D:55:ALA:HB3   | 2.03                     | 0.40              |
| 4:H:34:TYR:CD2   | 4:H:63:VAL:HB    | 2.56                     | 0.40              |
| 4:H:98:LEU:O     | 4:H:100:PRO:HD3  | 2.21                     | 0.40              |
| 5:I:156:DG:H2''  | 5:I:157:DA:H8    | 1.86                     | 0.40              |
| 6:J:142:DC:H2''  | 6:J:143:DT:C6    | 2.56                     | 0.40              |
| 7:U:147:TRP:O    | 7:U:517:LEU:HD11 | 2.21                     | 0.40              |
| 7:U:189:ILE:HA   | 7:U:196:PHE:HE2  | 1.86                     | 0.40              |
| 7:U:299:LEU:HD23 | 7:U:376:ASP:OD1  | 2.22                     | 0.40              |
| 7:U:342:VAL:C    | 7:U:344:PRO:HD3  | 2.47                     | 0.40              |
| 7:U:696:TYR:HA   | 7:U:699:ALA:HB3  | 2.04                     | 0.40              |
| 3:Q:59:THR:HG23  | 3:Q:60:ALA:N     | 2.37                     | 0.40              |
| 8:V:226:GLY:HA2  | 9:V:1201:ADP:O1A | 2.22                     | 0.40              |
| 8:V:629:ASP:OD1  | 8:V:630:ASN:N    | 2.55                     | 0.40              |
| 3:C:91:GLU:HG2   | 3:C:92:GLU:H     | 1.85                     | 0.40              |
| 4:D:99:LEU:HA    | 4:D:100:PRO:HD3  | 1.87                     | 0.40              |
| 1:E:97:GLU:HA    | 1:E:100:LEU:CG   | 2.52                     | 0.40              |
| 2:F:26:ILE:CD1   | 2:F:55:ARG:HB3   | 2.51                     | 0.40              |
| 5:I:317:DG:N2    | 6:J:-1:DG:C2     | 2.90                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:J:-6:DA:H2''   | 6:J:-5:DT:OP2    | 2.22                     | 0.40              |
| 6:J:79:DT:H1'    | 6:J:80:DA:C8     | 2.57                     | 0.40              |
| 7:U:175:PRO:HD2  | 7:U:217:GLY:HA2  | 2.02                     | 0.40              |
| 7:U:214:LEU:HD13 | 7:U:222:SER:HB2  | 2.02                     | 0.40              |
| 7:U:266:PHE:CD2  | 7:U:301:ARG:HB3  | 2.57                     | 0.40              |
| 3:M:71:ARG:NH1   | 4:N:49:THR:OG1   | 2.50                     | 0.40              |
| 1:O:129:ARG:HA   | 1:O:134:ARG:CB   | 2.51                     | 0.40              |
| 8:V:237:TYR:HA   | 8:V:241:ILE:HD13 | 2.02                     | 0.40              |
| 8:V:971:TYR:CE2  | 8:V:978:LEU:HA   | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | A     | 96/136 (71%)  | 91 (95%)   | 5 (5%)  | 0        | 100         | 100 |
| 1   | E     | 93/136 (68%)  | 89 (96%)   | 4 (4%)  | 0        | 100         | 100 |
| 1   | K     | 96/136 (71%)  | 93 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 1   | O     | 93/136 (68%)  | 90 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 2   | B     | 80/103 (78%)  | 76 (95%)   | 4 (5%)  | 0        | 100         | 100 |
| 2   | F     | 84/103 (82%)  | 83 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 2   | L     | 86/103 (84%)  | 82 (95%)   | 4 (5%)  | 0        | 100         | 100 |
| 2   | P     | 78/103 (76%)  | 75 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 3   | C     | 105/130 (81%) | 104 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 3   | G     | 105/130 (81%) | 105 (100%) | 0       | 0        | 100         | 100 |
| 3   | M     | 105/130 (81%) | 101 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 3   | Q     | 105/130 (81%) | 102 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 4   | D     | 91/126 (72%)  | 87 (96%)   | 4 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 4   | H     | 91/126 (72%)    | 90 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 4   | N     | 91/126 (72%)    | 85 (93%)   | 6 (7%)   | 0        | 100         | 100 |
| 4   | R     | 91/126 (72%)    | 88 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 7   | U     | 586/624 (94%)   | 523 (89%)  | 62 (11%) | 1 (0%)   | 43          | 77  |
| 8   | V     | 780/1062 (73%)  | 713 (91%)  | 67 (9%)  | 0        | 100         | 100 |
| All | All   | 2856/3666 (78%) | 2677 (94%) | 178 (6%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | U     | 328 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | A     | 84/111 (76%) | 84 (100%) | 0        | 100         | 100 |
| 1   | E     | 82/111 (74%) | 82 (100%) | 0        | 100         | 100 |
| 1   | K     | 84/111 (76%) | 84 (100%) | 0        | 100         | 100 |
| 1   | O     | 82/111 (74%) | 82 (100%) | 0        | 100         | 100 |
| 2   | B     | 67/79 (85%)  | 57 (85%)  | 10 (15%) | 3           | 13  |
| 2   | F     | 67/79 (85%)  | 67 (100%) | 0        | 100         | 100 |
| 2   | L     | 72/79 (91%)  | 72 (100%) | 0        | 100         | 100 |
| 2   | P     | 64/79 (81%)  | 64 (100%) | 0        | 100         | 100 |
| 3   | C     | 81/102 (79%) | 81 (100%) | 0        | 100         | 100 |
| 3   | G     | 82/102 (80%) | 82 (100%) | 0        | 100         | 100 |
| 3   | M     | 81/102 (79%) | 81 (100%) | 0        | 100         | 100 |
| 3   | Q     | 82/102 (80%) | 82 (100%) | 0        | 100         | 100 |
| 4   | D     | 77/106 (73%) | 77 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 4   | H     | 79/106 (74%)    | 79 (100%)   | 0        | 100         | 100 |
| 4   | N     | 77/106 (73%)    | 77 (100%)   | 0        | 100         | 100 |
| 4   | R     | 79/106 (74%)    | 79 (100%)   | 0        | 100         | 100 |
| 7   | U     | 541/571 (95%)   | 541 (100%)  | 0        | 100         | 100 |
| 8   | V     | 724/959 (76%)   | 724 (100%)  | 0        | 100         | 100 |
| All | All   | 2505/3122 (80%) | 2495 (100%) | 10 (0%)  | 81          | 83  |

All (10) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 79  | LYS  |
| 2   | B     | 81  | VAL  |
| 2   | B     | 84  | MET  |
| 2   | B     | 88  | TYR  |
| 2   | B     | 90  | LEU  |
| 2   | B     | 91  | LYS  |
| 2   | B     | 92  | ARG  |
| 2   | B     | 93  | GLN  |
| 2   | B     | 95  | ARG  |
| 2   | B     | 96  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 93  | GLN  |
| 1   | A     | 108 | ASN  |
| 1   | A     | 113 | HIS  |
| 2   | B     | 27  | GLN  |
| 3   | C     | 31  | HIS  |
| 3   | C     | 68  | ASN  |
| 4   | D     | 92  | GLN  |
| 1   | E     | 93  | GLN  |
| 2   | F     | 25  | ASN  |
| 2   | F     | 93  | GLN  |
| 4   | H     | 81  | ASN  |
| 7   | U     | 206 | GLN  |
| 7   | U     | 452 | GLN  |
| 7   | U     | 463 | HIS  |
| 7   | U     | 545 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 7   | U     | 573  | GLN  |
| 7   | U     | 613  | HIS  |
| 7   | U     | 682  | ASN  |
| 7   | U     | 688  | ASN  |
| 7   | U     | 722  | GLN  |
| 2   | L     | 64   | ASN  |
| 4   | N     | 44   | GLN  |
| 4   | N     | 92   | GLN  |
| 1   | O     | 85   | GLN  |
| 3   | Q     | 82   | HIS  |
| 4   | R     | 46   | HIS  |
| 4   | R     | 79   | HIS  |
| 8   | V     | 230  | GLN  |
| 8   | V     | 258  | ASN  |
| 8   | V     | 272  | ASN  |
| 8   | V     | 402  | HIS  |
| 8   | V     | 471  | GLN  |
| 8   | V     | 496  | HIS  |
| 8   | V     | 500  | ASN  |
| 8   | V     | 526  | GLN  |
| 8   | V     | 554  | HIS  |
| 8   | V     | 607  | GLN  |
| 8   | V     | 648  | GLN  |
| 8   | V     | 808  | GLN  |
| 8   | V     | 810  | GLN  |
| 8   | V     | 853  | GLN  |
| 8   | V     | 866  | GLN  |
| 8   | V     | 933  | ASN  |
| 8   | V     | 1051 | GLN  |
| 8   | V     | 1058 | ASN  |

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 10  | BEF  | V     | 1202 | -    | 0,3,3        | -    | -           | -           |      |             |
| 9   | ADP  | V     | 1201 | 11   | 27,29,29     | 1.36 | 4 (14%)     | 42,45,45    | 1.96 | 10 (23%)    |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 9   | ADP  | V     | 1201 | 11   | -       | 4/16/32/32 | 0/3/3/3 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | V     | 1201 | ADP  | C5-C4 | 4.45  | 1.47        | 1.39     |
| 9   | V     | 1201 | ADP  | C5-C6 | 2.73  | 1.48        | 1.41     |
| 9   | V     | 1201 | ADP  | C8-N7 | 2.41  | 1.36        | 1.31     |
| 9   | V     | 1201 | ADP  | C5-N7 | -2.12 | 1.35        | 1.39     |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 9   | V     | 1201 | ADP  | C5-C4-N3  | -5.86 | 119.11      | 126.75   |
| 9   | V     | 1201 | ADP  | N3-C4-N9  | 4.60  | 134.66      | 127.08   |
| 9   | V     | 1201 | ADP  | PA-O3A-PB | -3.90 | 119.45      | 132.83   |
| 9   | V     | 1201 | ADP  | C2-N3-C4  | 3.81  | 120.75      | 111.75   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 9   | V     | 1201 | ADP  | C4-C5-N7 | -3.21 | 106.70      | 110.62   |
| 9   | V     | 1201 | ADP  | N3-C2-N1 | -3.20 | 123.60      | 128.60   |
| 9   | V     | 1201 | ADP  | C4-N9-C8 | 2.76  | 108.72      | 105.73   |
| 9   | V     | 1201 | ADP  | C5-N7-C8 | 2.58  | 107.18      | 103.51   |
| 9   | V     | 1201 | ADP  | C6-C5-N7 | 2.35  | 136.39      | 132.02   |
| 9   | V     | 1201 | ADP  | N9-C8-N7 | -2.01 | 111.17      | 113.91   |

There are no chirality outliers.

All (4) torsion outliers are listed below:

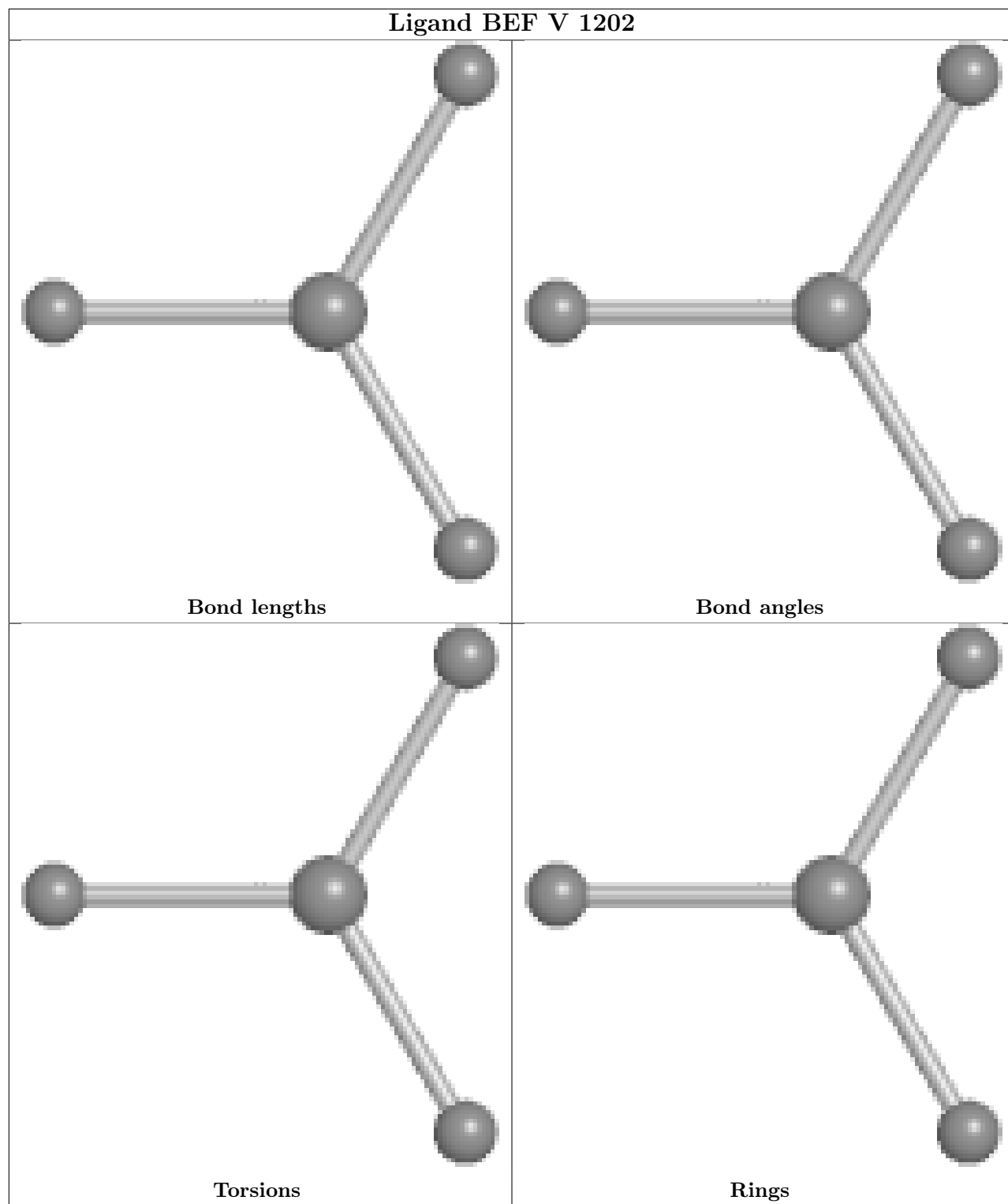
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 9   | V     | 1201 | ADP  | O4'-C4'-C5'-O5' |
| 9   | V     | 1201 | ADP  | C3'-C4'-C5'-O5' |
| 9   | V     | 1201 | ADP  | PB-O3A-PA-O1A   |
| 9   | V     | 1201 | ADP  | PB-O3A-PA-O2A   |

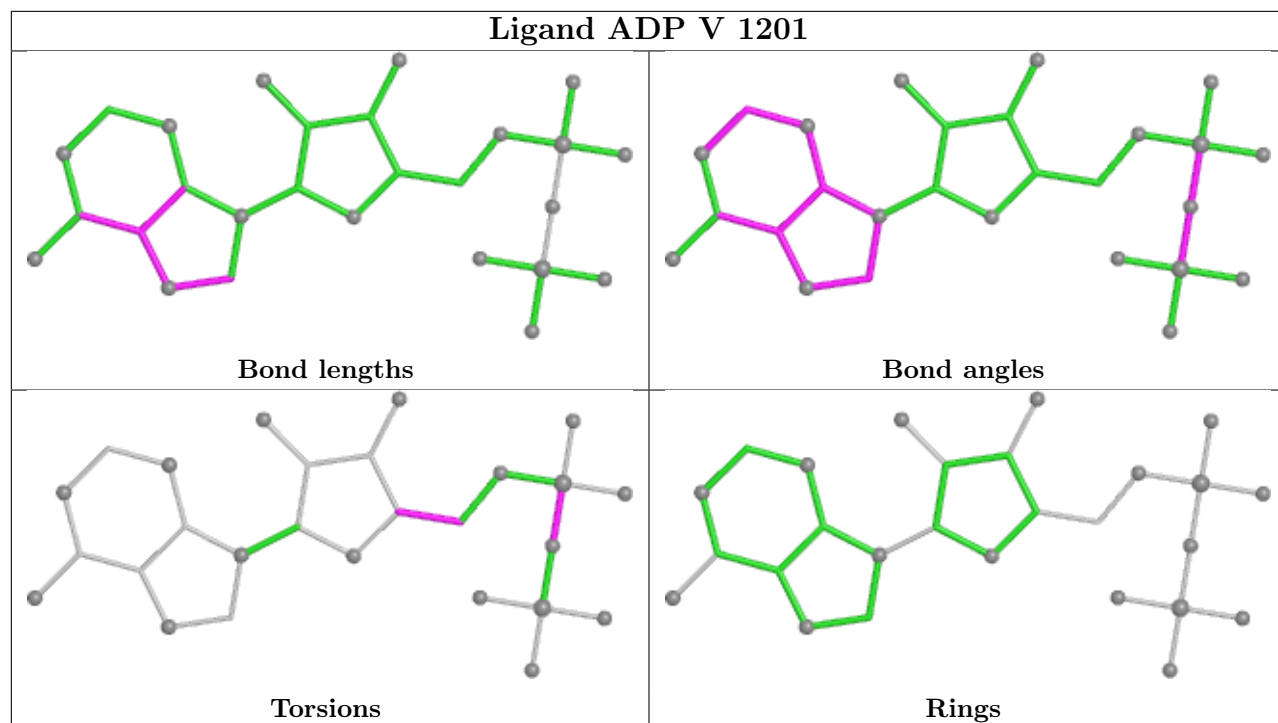
There are no ring outliers.

2 monomers are involved in 8 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 10  | V     | 1202 | BEF  | 3       | 0            |
| 9   | V     | 1201 | ADP  | 6       | 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.

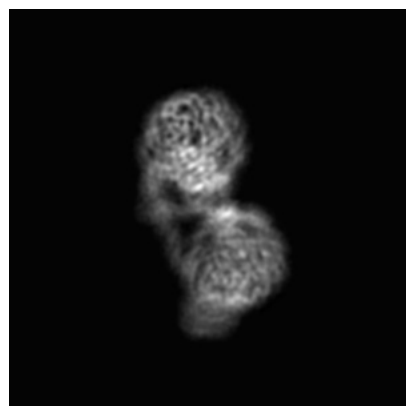
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32992. These allow visual inspection of the internal detail of the map and identification of artifacts.

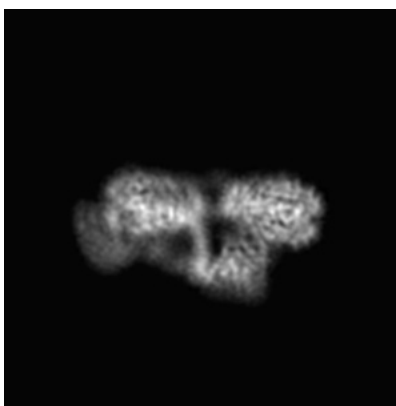
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

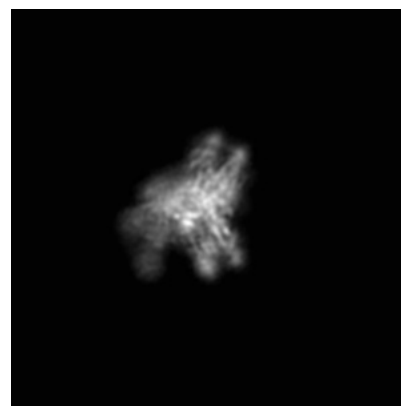
#### 6.1.1 Primary map



X

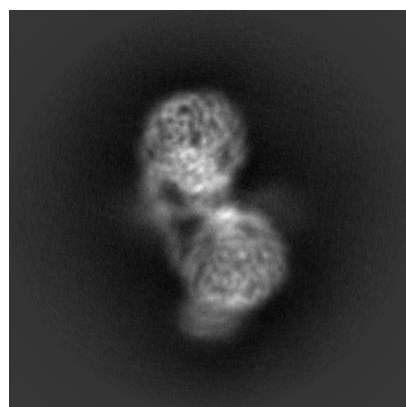


Y

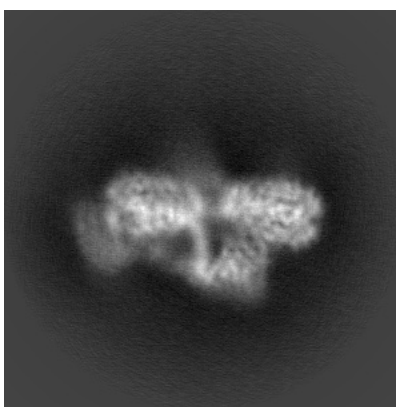


Z

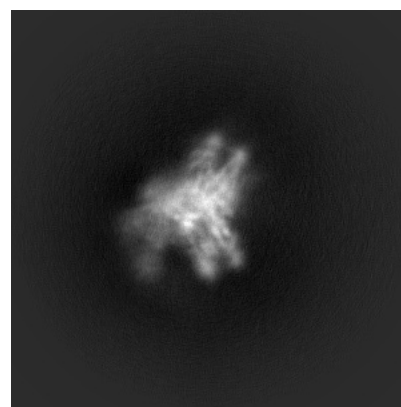
#### 6.1.2 Raw map



X



Y

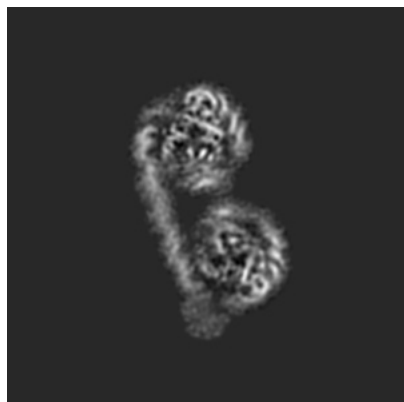


Z

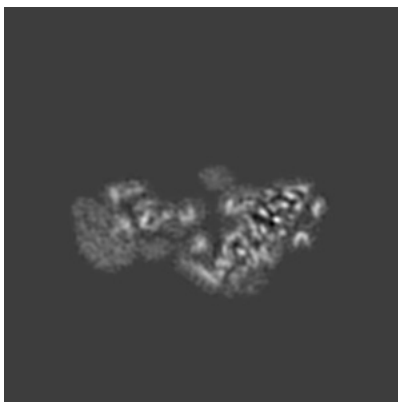
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 180

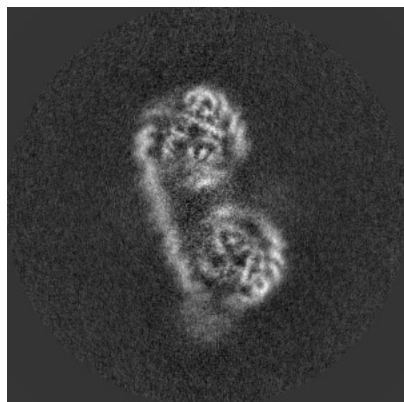


Y Index: 180

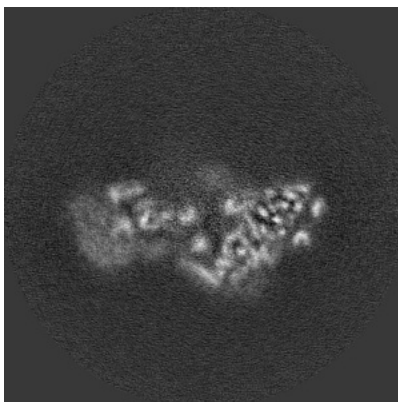


Z Index: 180

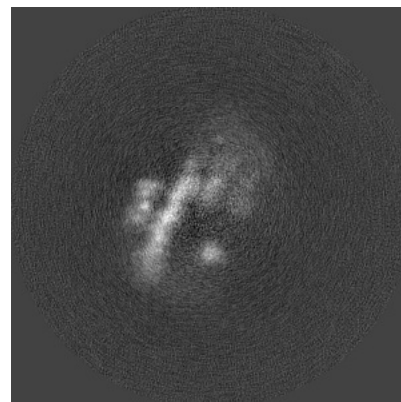
### 6.2.2 Raw map



X Index: 180



Y Index: 180

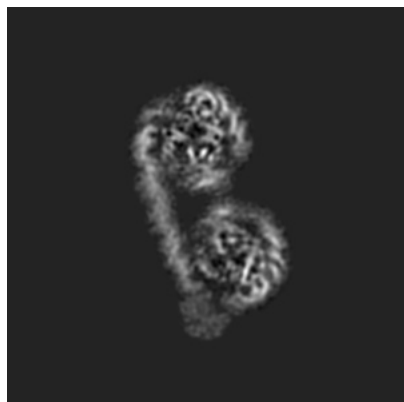


Z Index: 180

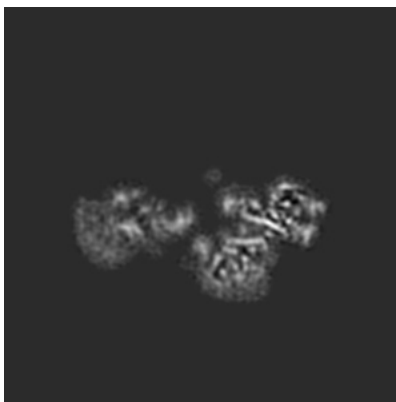
The images above show central slices of the map in three orthogonal directions.

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

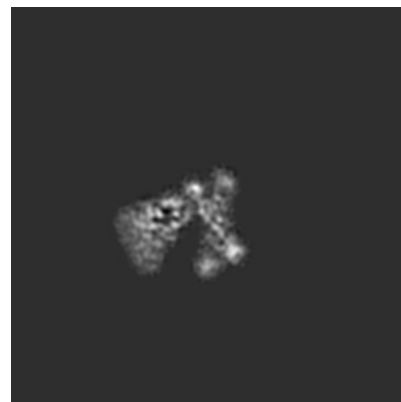
### 6.3.1 Primary map



X Index: 179

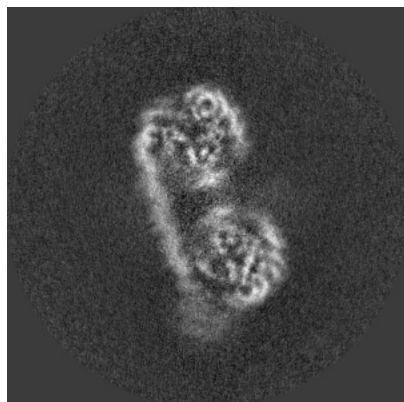


Y Index: 174



Z Index: 217

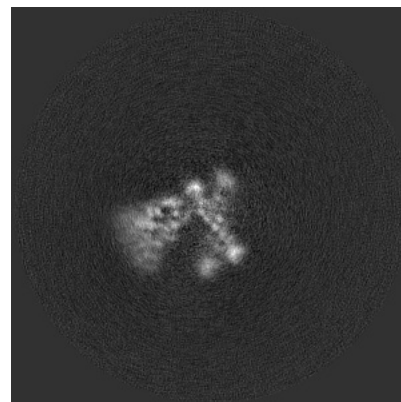
### 6.3.2 Raw map



X Index: 178



Y Index: 174

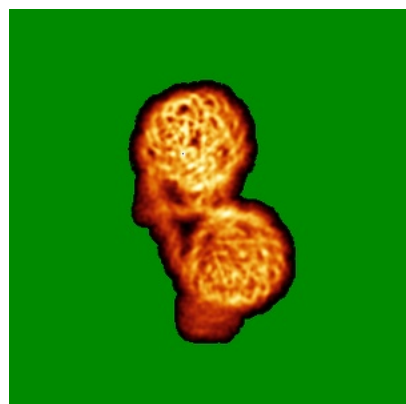


Z Index: 218

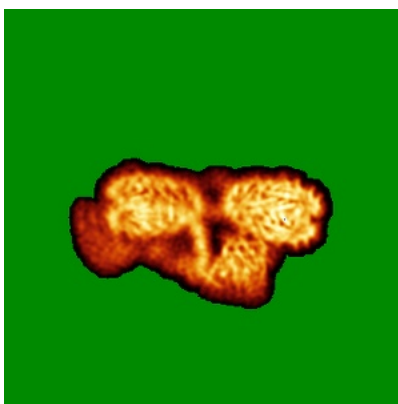
The images above show the largest variance slices of the map in three orthogonal directions.

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

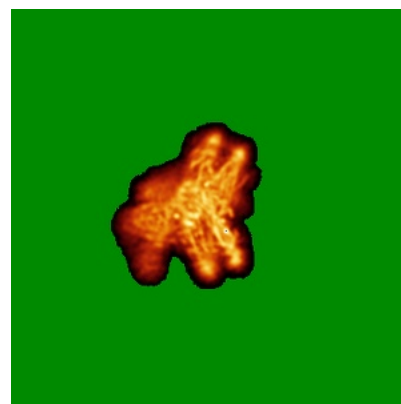
### 6.4.1 Primary map



X

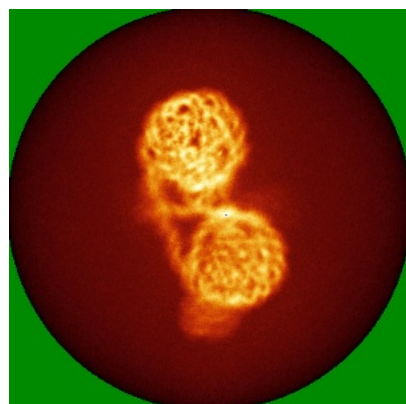


Y

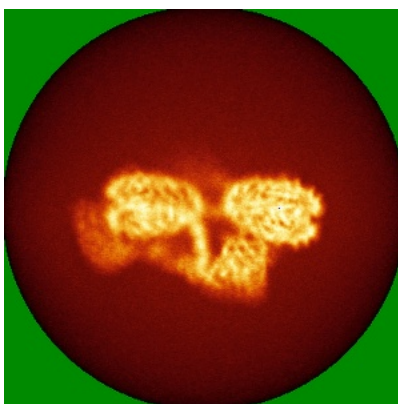


Z

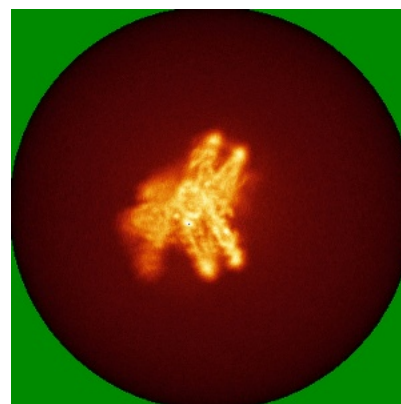
### 6.4.2 Raw map



X



Y



Z

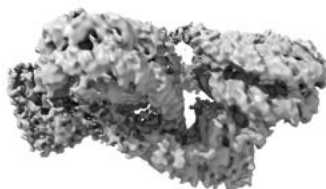
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

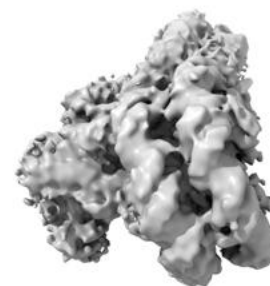
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0048. 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



X



Y



Z

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.

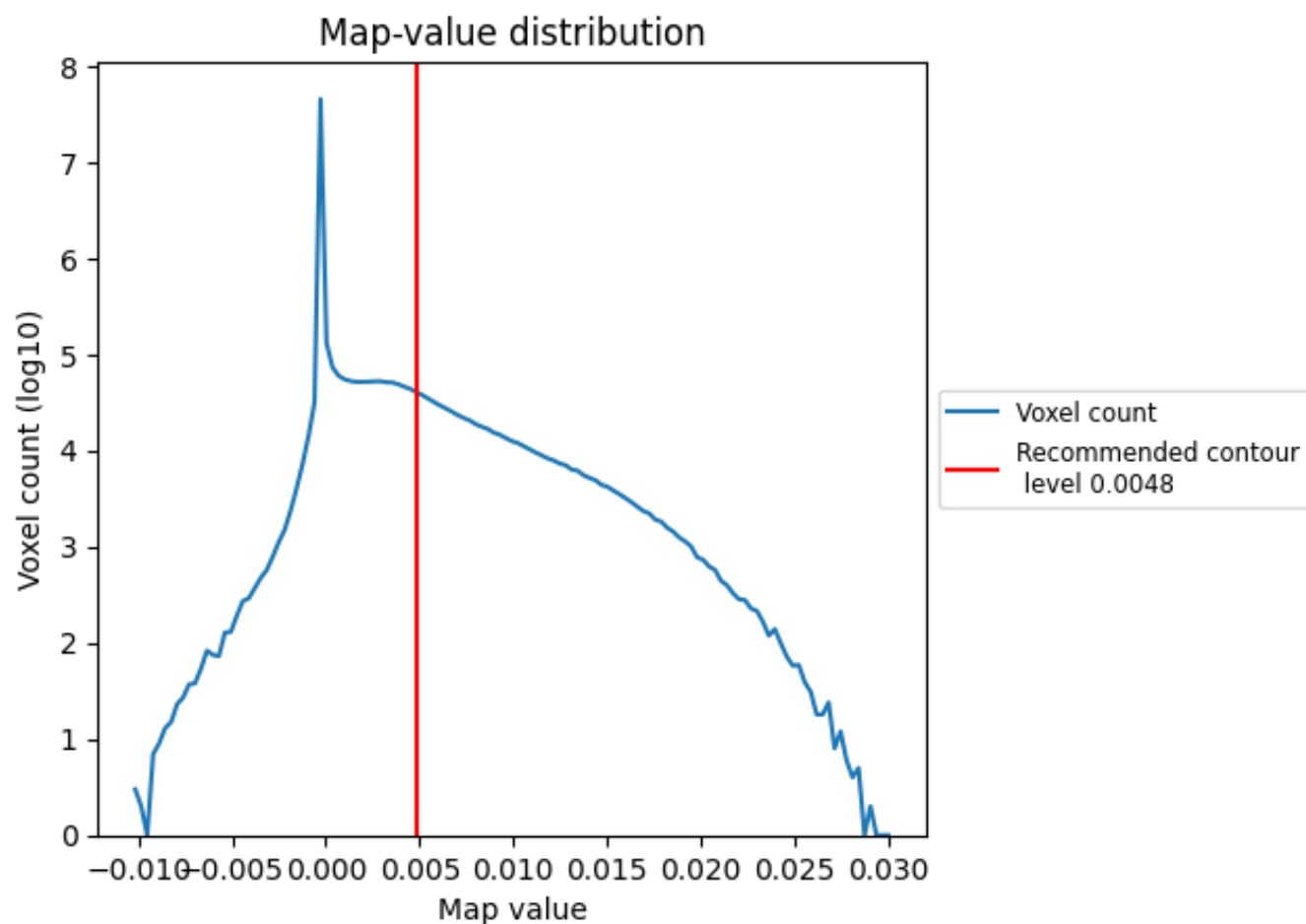
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

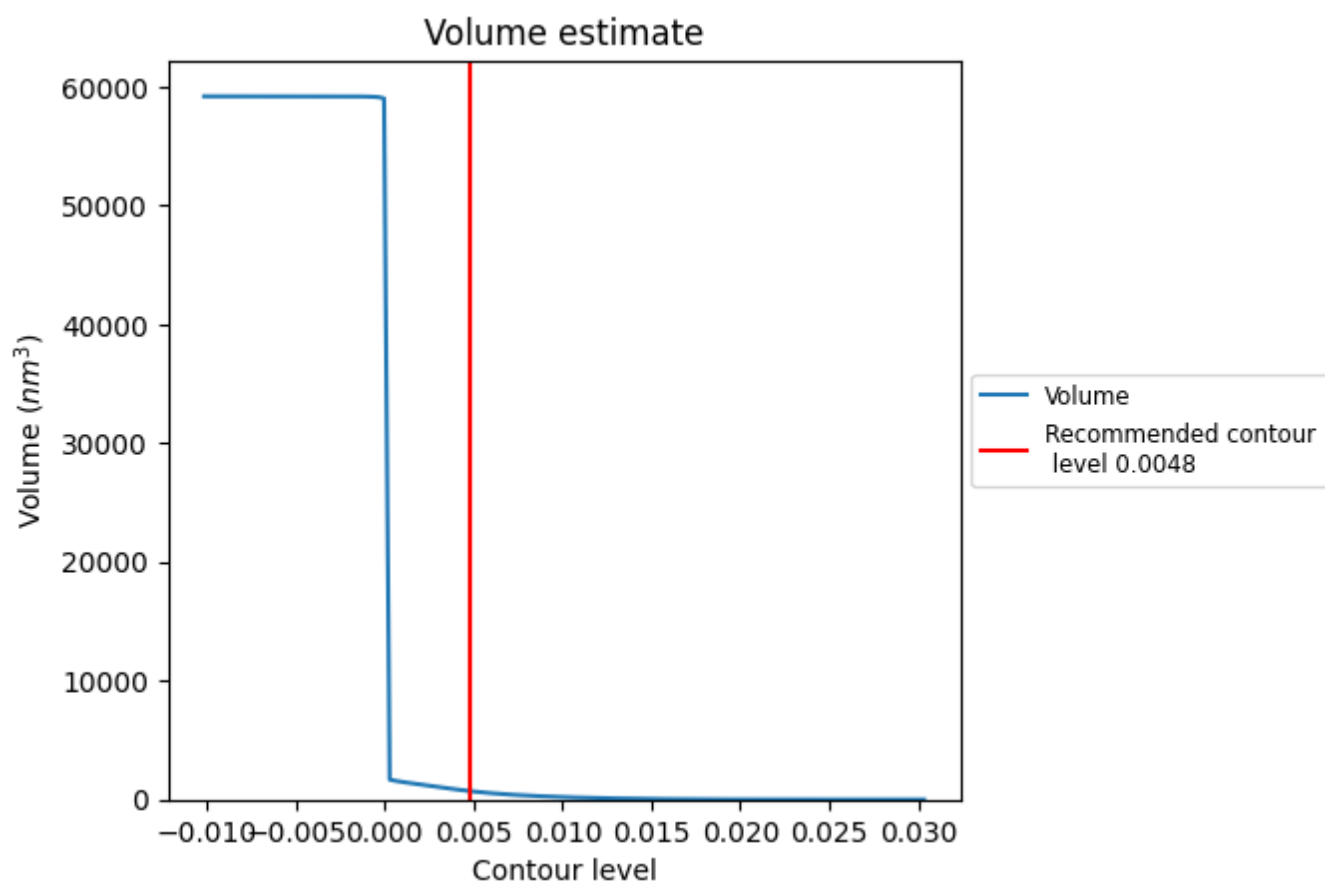
This section contains the results of statistical analysis of the map.

### 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.

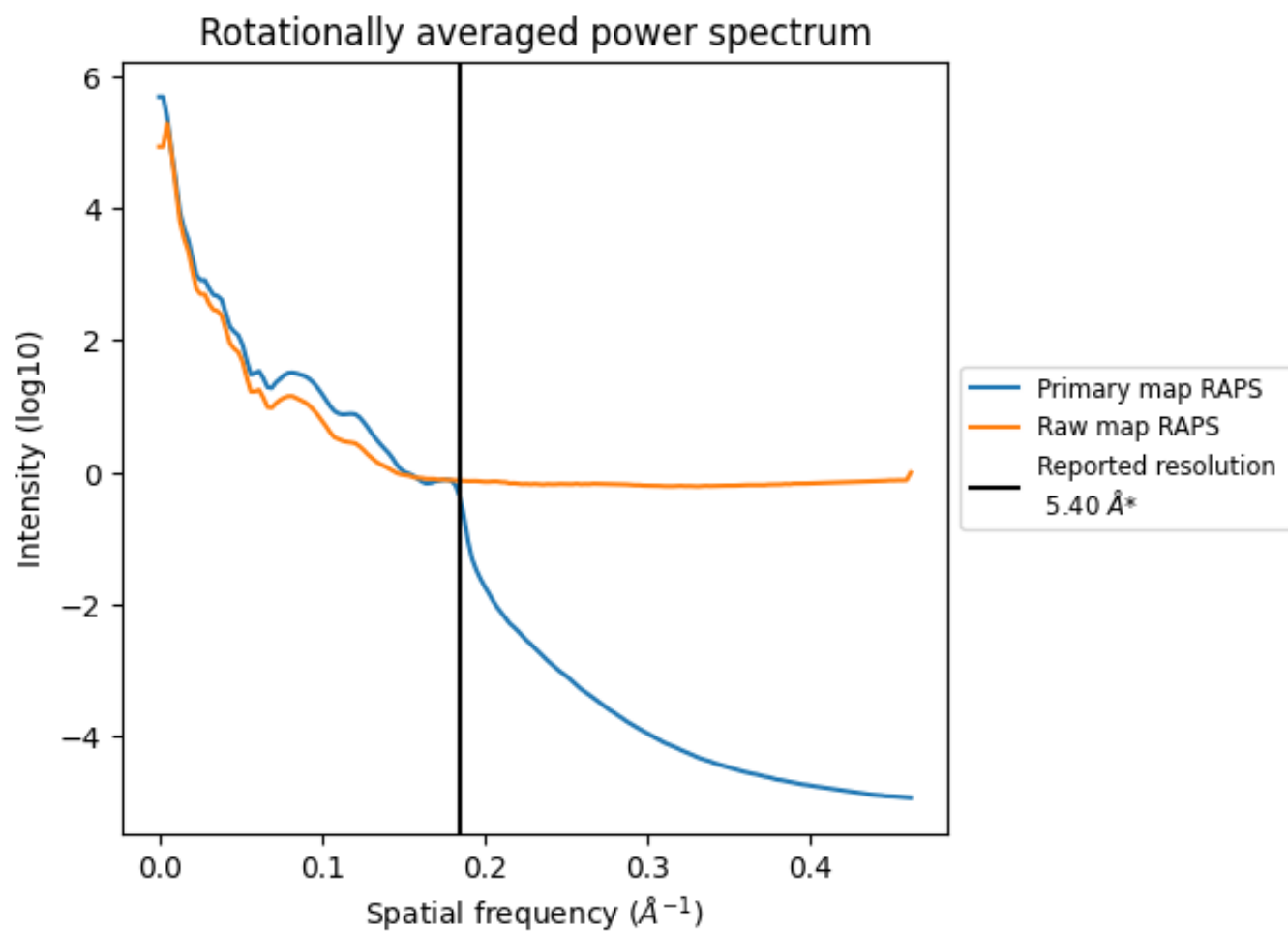
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 711 nm<sup>3</sup>; this corresponds to an approximate mass of 643 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 ⓘ

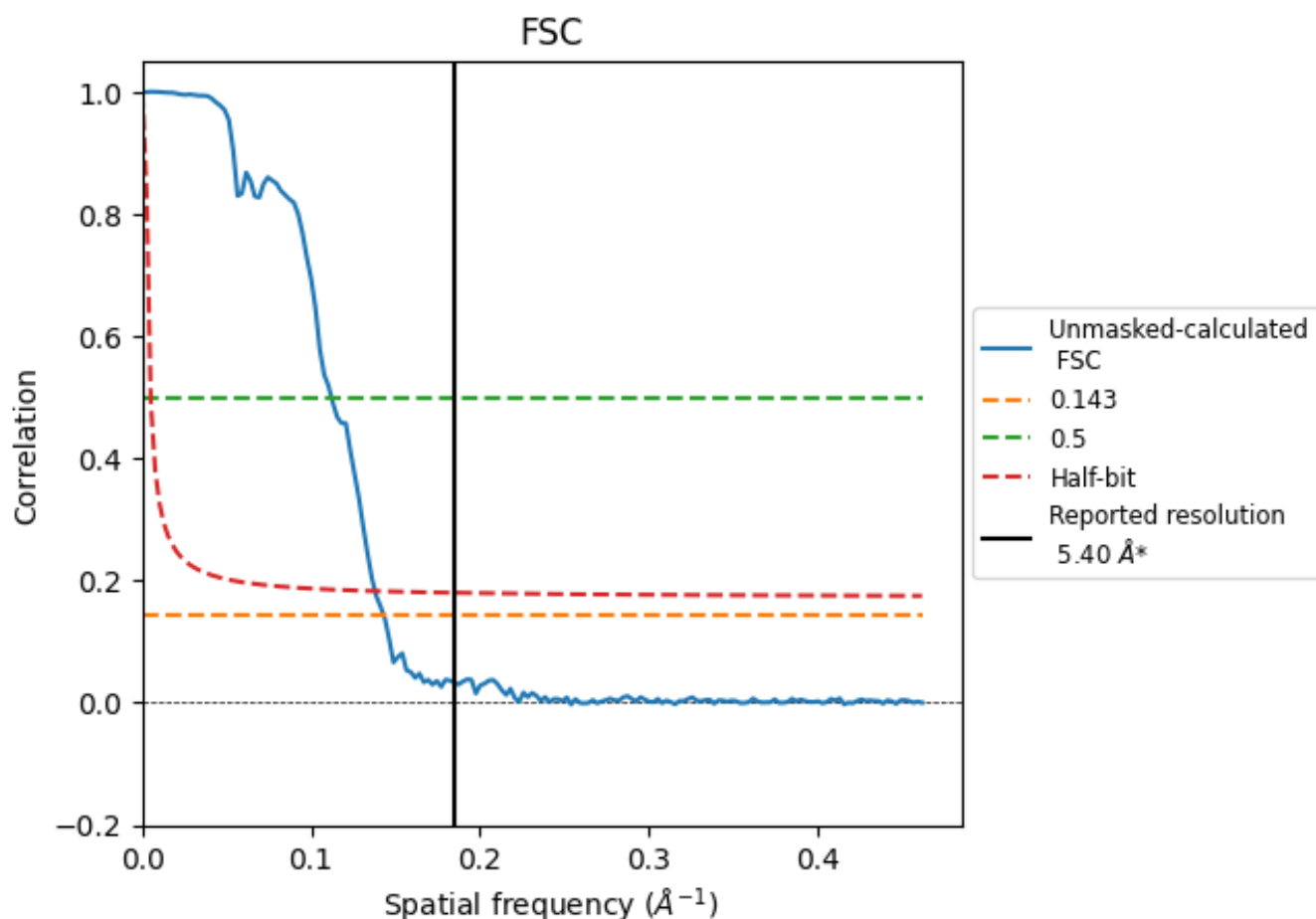


\*Reported resolution corresponds to spatial frequency of 0.185 Å<sup>-1</sup>

## 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  $0.185 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

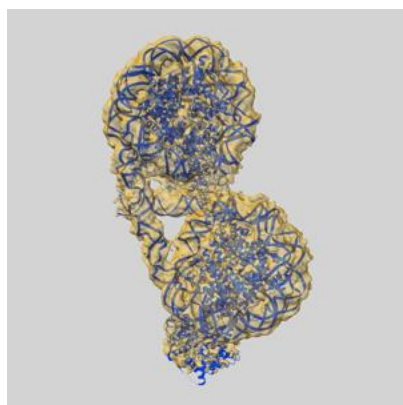
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 5.40                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 6.99                               | 8.92 | 7.25     |

\*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 6.99 differs from the reported value 5.4 by more than 10 %

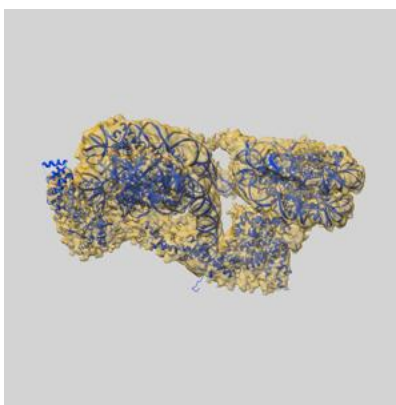
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32992 and PDB model 7X3T. Per-residue inclusion information can be found in section [3](#) on page [8](#).

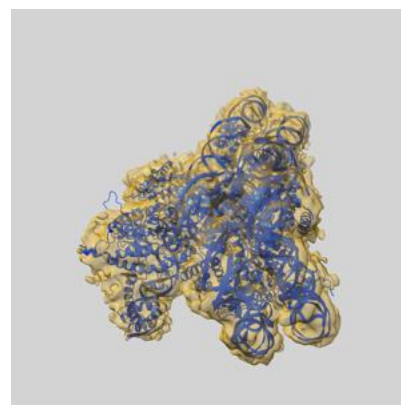
### 9.1 Map-model overlay [i](#)



X



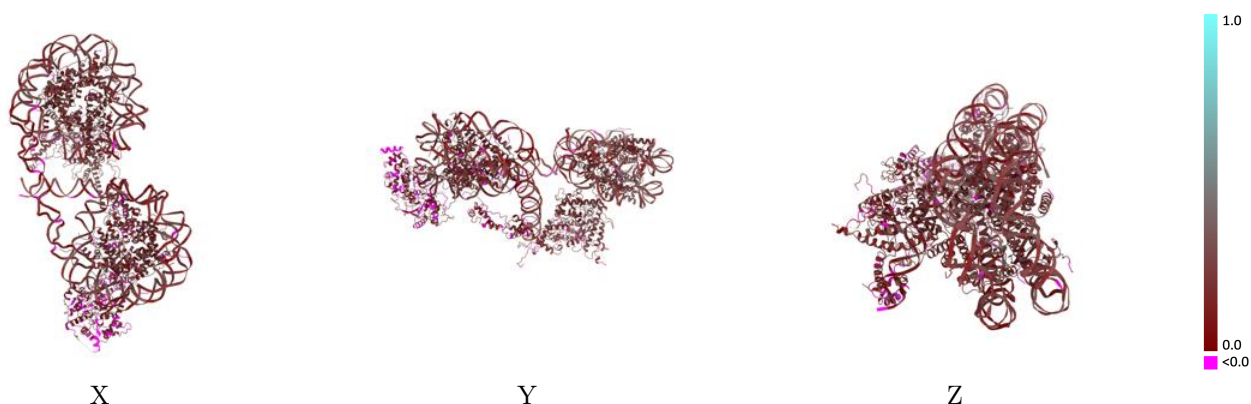
Y



Z

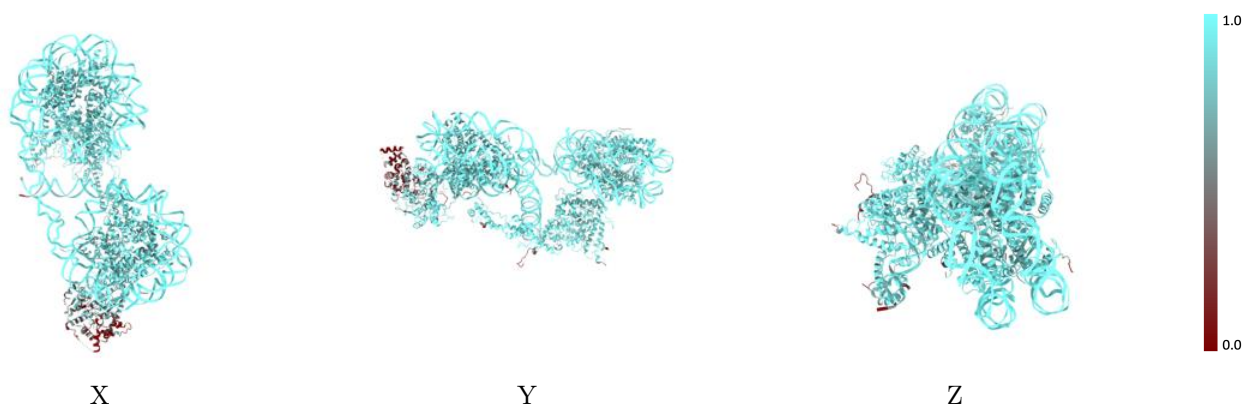
The images above show the 3D surface view of the map at the recommended contour level 0.0048 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



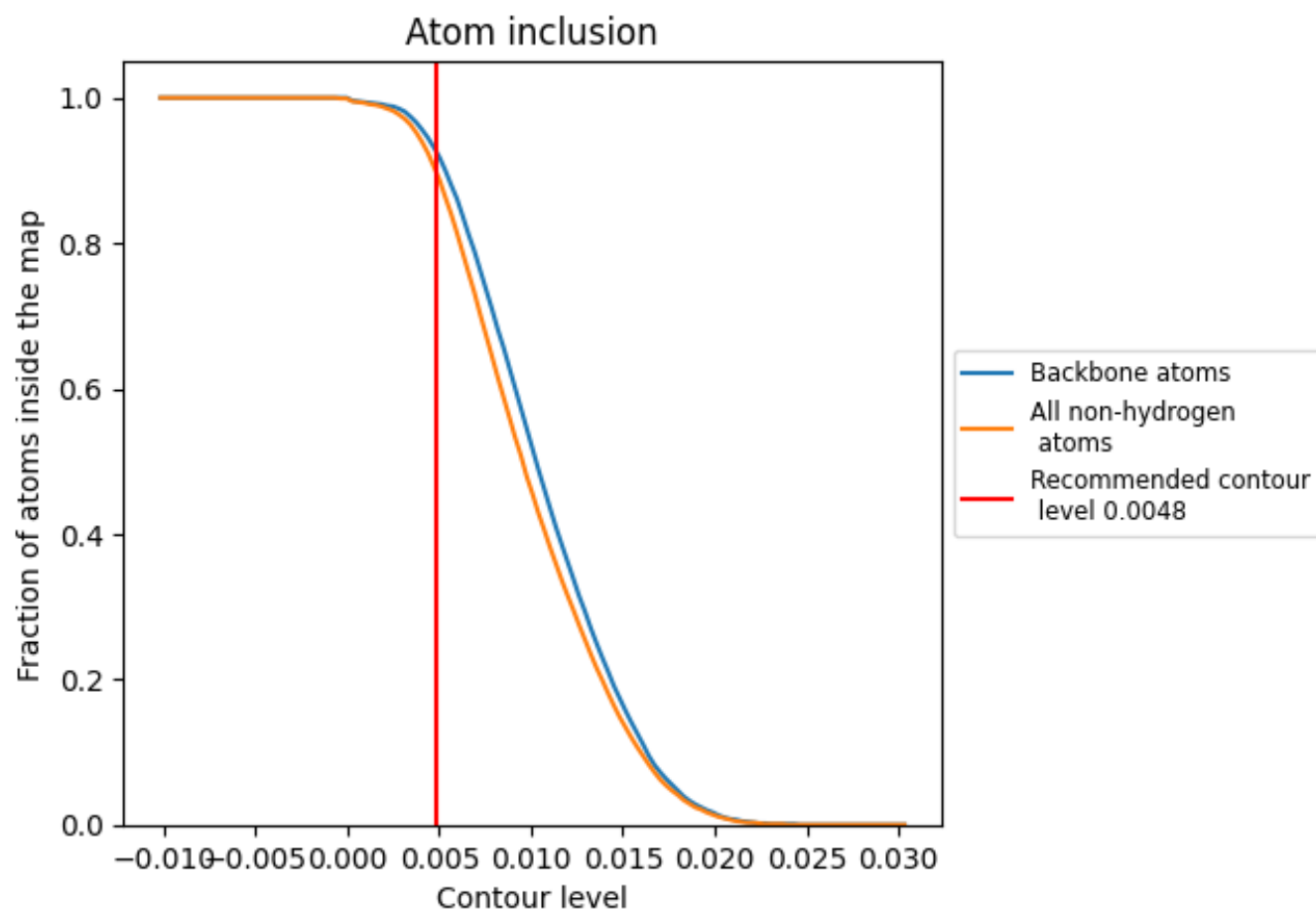
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0048).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.0048) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9000   |  0.1920   |
| A     |  0.9470   |  0.2150   |
| B     |  0.9170   |  0.2360   |
| C     |  0.9130   |  0.2480   |
| D     |  0.9290   |  0.2540   |
| E     |  0.9150   |  0.2110   |
| F     |  0.8830   |  0.2310   |
| G     |  0.9320   |  0.2430   |
| H     |  0.9150   |  0.2410   |
| I     |  0.9720   |  0.2000   |
| J     |  0.9720   |  0.2020   |
| K     |  0.8910   |  0.2100   |
| L     |  0.8980   |  0.2230   |
| M     |  0.8920   |  0.2070   |
| N     |  0.9030  |  0.2150  |
| O     |  0.9320 |  0.1900 |
| P     |  0.9290 |  0.1870 |
| Q     |  0.8920 |  0.2050 |
| R     |  0.9360 |  0.2220 |
| U     |  0.9200 |  0.1950 |
| V     |  0.7080 |  0.1200 |

