



## Full wwPDB EM Validation Report ⓘ

Aug 7, 2026 – 01:45 AM JST

PDB ID : 8X19 / pdb\_00008x19  
EMDB ID : EMD-37988  
Title : Structure of nucleosome-bound SRCAP-C in the ADP-BeFx-bound state  
Authors : Yu, J.; Wang, Q.; Yu, Z.; Li, W.; Wang, L.; Xu, Y.  
Deposited on : 2023-11-06  
Resolution : 3.20 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:

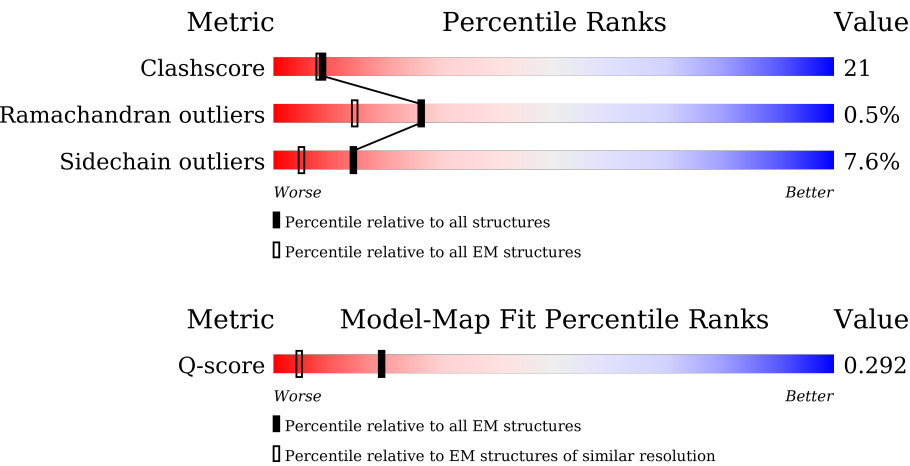
EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 i

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

The reported resolution of this entry is 3.20 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                       | 15020 ( 2.70 - 3.70 )                                    |

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     | 130    |                  |
| 1   | E     | 130    |                  |
| 2   | B     | 126    |                  |
| 2   | F     | 126    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | C     | 136    |                  |
| 3   | G     | 136    |                  |
| 4   | D     | 103    |                  |
| 4   | H     | 103    |                  |
| 5   | I     | 3230   |                  |
| 6   | J     | 364    |                  |
| 7   | K     | 396    |                  |
| 8   | L     | 154    |                  |
| 9   | M     | 456    |                  |
| 9   | O     | 456    |                  |
| 9   | Q     | 456    |                  |
| 10  | N     | 463    |                  |
| 10  | P     | 463    |                  |
| 10  | R     | 463    |                  |
| 11  | S     | 375    |                  |
| 11  | U     | 375    |                  |
| 12  | T     | 429    |                  |
| 13  | V     | 467    |                  |
| 14  | W     | 227    |                  |
| 15  | X     | 147    |                  |
| 16  | Y     | 147    |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 19  | BEF  | I     | 3303 | -         | -        | X       | -                |

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 56704 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 H2A type 1-C.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 1   | A     | 108      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 833   | 525 | 165 | 143 |         |       |
| 1   | E     | 105      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 808   | 510 | 158 | 140 |         |       |

- Molecule 2 is a protein called Histone H2B type 1-C/E/F/G/I.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | B     | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 755   | 473 | 138 | 142 | 2 |         |       |
| 2   | F     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 736   | 461 | 134 | 139 | 2 |         |       |

- Molecule 3 is a protein called Histone H3.1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | C     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 779   | 491 | 148 | 136 | 4 |         |       |
| 3   | G     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 801   | 505 | 155 | 137 | 4 |         |       |

- Molecule 4 is a protein called Histone H4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | D     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 646   | 407 | 126 | 112 | 1 |         |       |
| 4   | H     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 638   | 401 | 125 | 111 | 1 |         |       |

- Molecule 5 is a protein called Helicase SRCAP.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 5   | I     | 864      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7122  | 4533 | 1314 | 1236 | 39 |         |       |

- Molecule 6 is a protein called Vacuolar protein sorting-associated protein 72 homolog.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | J     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1350  | 846 | 260 | 239 | 5 |         |       |

- Molecule 7 is a protein called Actin-related protein 6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | K     | 394      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3209  | 2054 | 526 | 611 | 18 |         |       |

- Molecule 8 is a protein called Zinc finger HIT domain-containing protein 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | L     | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 893   | 546 | 173 | 165 | 9 |         |       |

- Molecule 9 is a protein called RuvB-like 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | M     | 418      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3213  | 2026 | 557 | 614 | 16 |         |       |
| 9   | O     | 435      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3339  | 2105 | 571 | 646 | 17 |         |       |
| 9   | Q     | 440      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3368  | 2121 | 579 | 651 | 17 |         |       |

- Molecule 10 is a protein called RuvB-like 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | N     | 411      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3185  | 1988 | 560 | 622 | 15 |         |       |
| 10  | P     | 427      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3287  | 2054 | 576 | 642 | 15 |         |       |
| 10  | R     | 424      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3293  | 2057 | 578 | 642 | 16 |         |       |

- Molecule 11 is a protein called Actin, cytoplasmic 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | S     | 375      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2925  | 1850 | 491 | 561 | 23 |         |       |
| 11  | U     | 359      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2802  | 1775 | 468 | 540 | 19 |         |       |

- Molecule 12 is a protein called Actin-like protein 6A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | T     | 403      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3146  | 1988 | 535 | 599 | 24 |         |       |

- Molecule 13 is a protein called DNA methyltransferase 1-associated protein 1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | V     | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1757  | 1117 | 327 | 309 | 4 |         |       |

- Molecule 14 is a protein called YEATS domain-containing protein 4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | W     | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1542  | 998 | 255 | 284 | 5 |         |       |

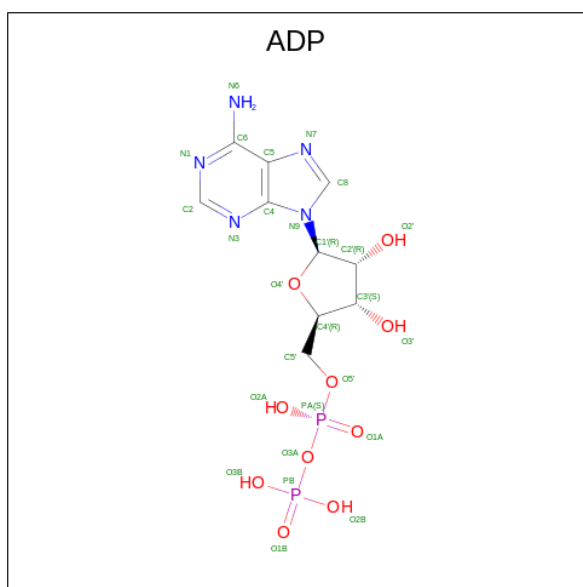
- Molecule 15 is a DNA chain called DNA (147-MER).

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 15  | X     | 147      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 3031  | 1435 | 572 | 878 | 146 |         |       |

- Molecule 16 is a DNA chain called DNA (147-MER).

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 16  | Y     | 147      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2990  | 1422 | 540 | 882 | 146 |         |       |

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

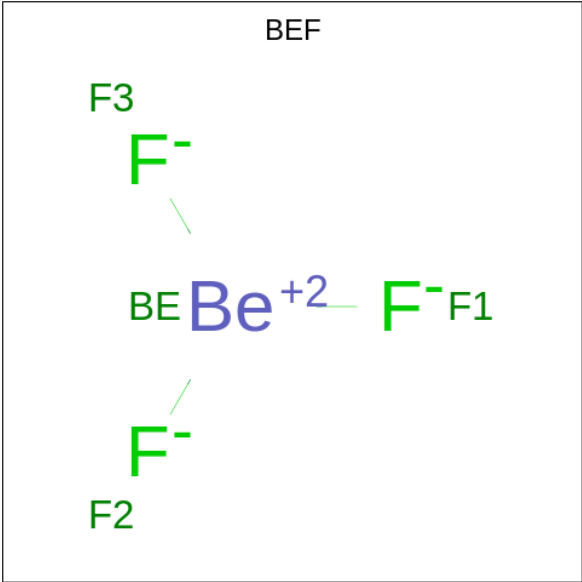


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 17  | I     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 17  | M     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 17  | N     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 17  | O     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 17  | P     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 17  | Q     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 17  | R     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

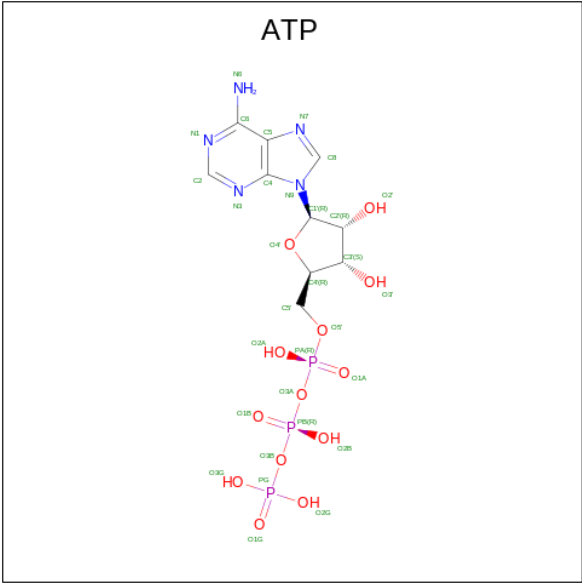
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 18  | I     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 19 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



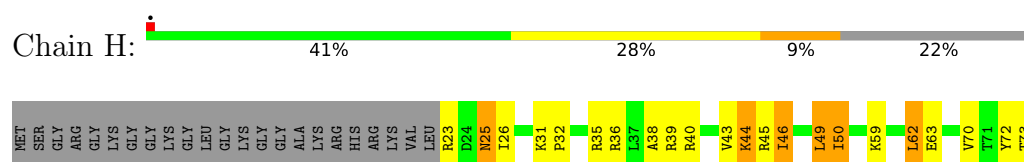
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
|     |       |          | Total | Be | F |         |
| 19  | I     | 1        | 4     | 1  | 3 | 0       |

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
|     |       |          | Total | C  | N | O  | P |         |
| 20  | T     | 1        | 31    | 10 | 5 | 13 | 3 | 0       |
| 20  | U     | 1        | 31    | 10 | 5 | 13 | 3 | 0       |

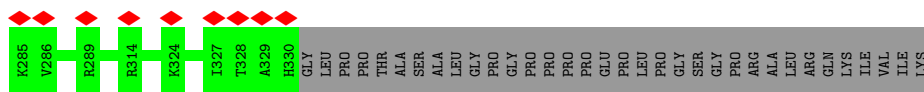




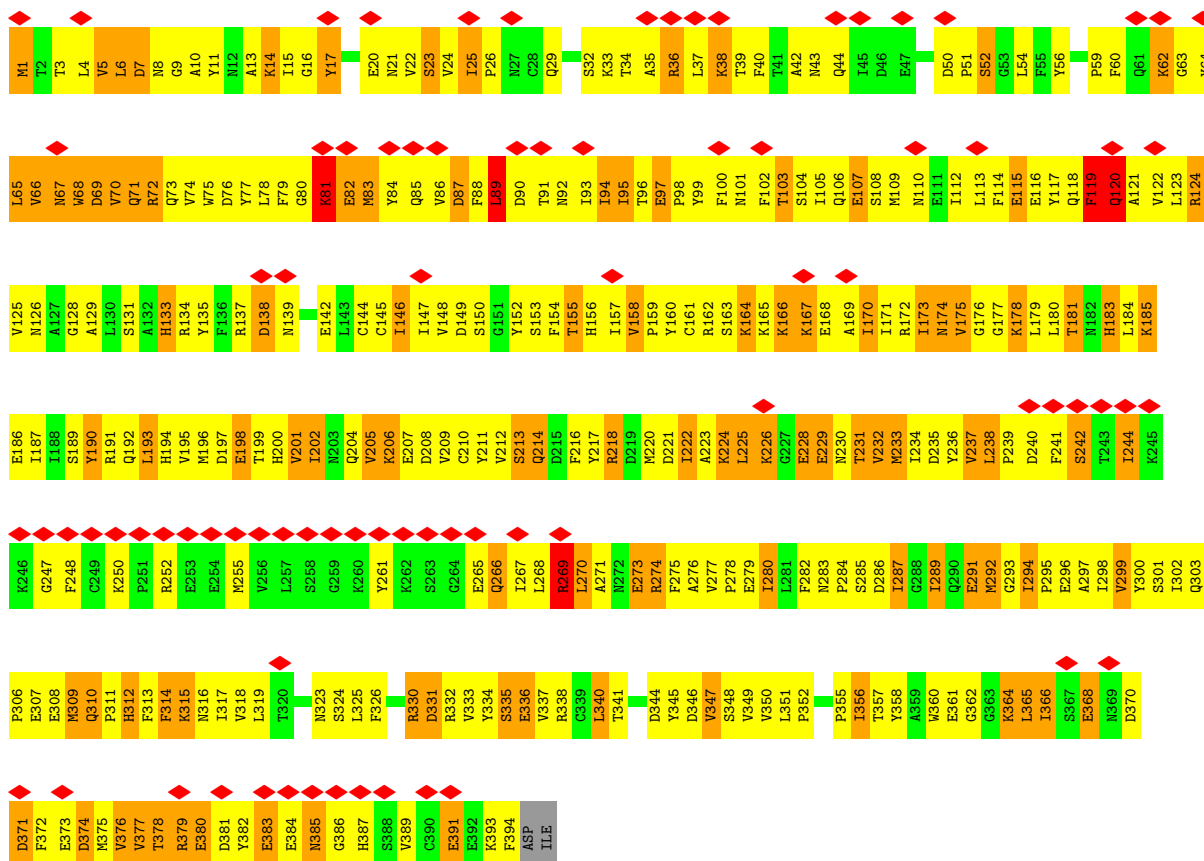
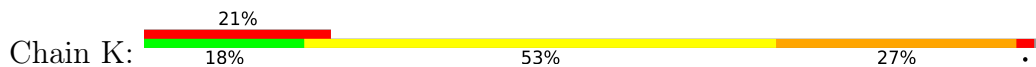




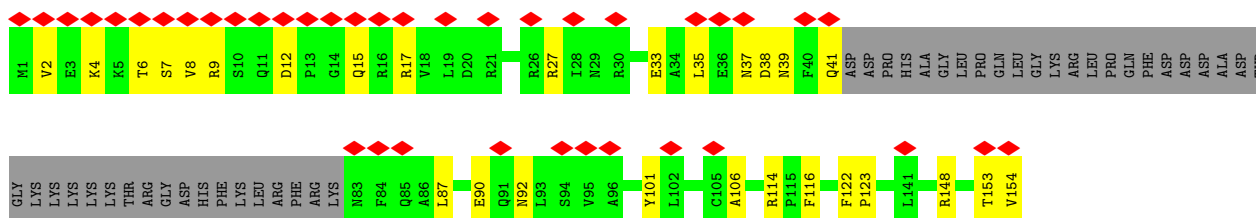




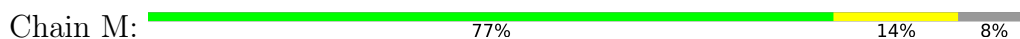
• Molecule 7: Actin-related protein 6

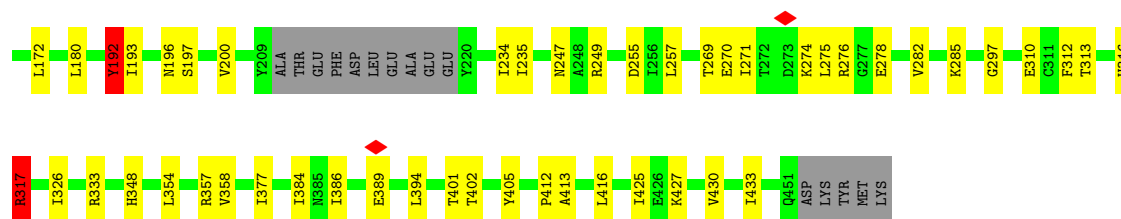


• Molecule 8: Zinc finger HIT domain-containing protein 1

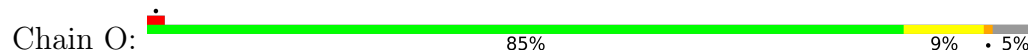


• Molecule 9: RuvB-like 1

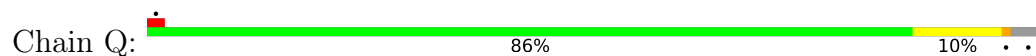




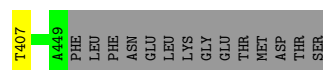
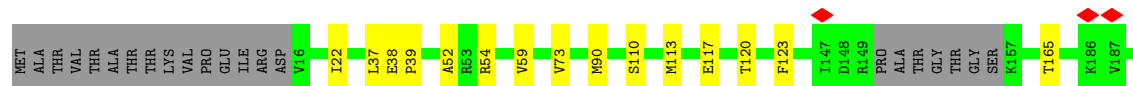
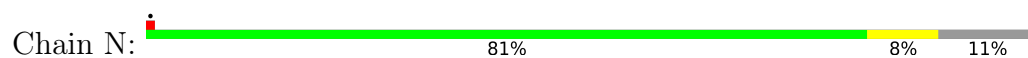
• Molecule 9: RuvB-like 1



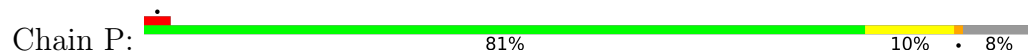
• Molecule 9: RuvB-like 1

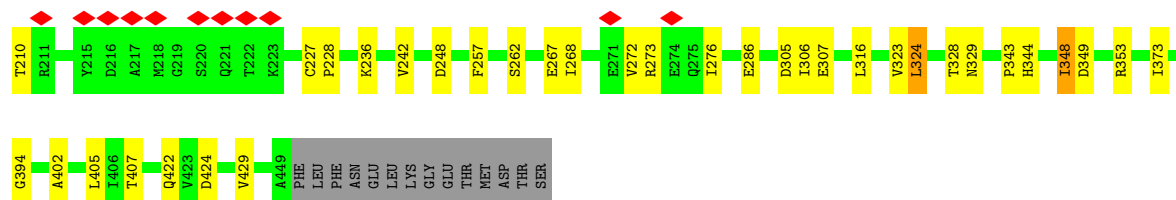


• Molecule 10: RuvB-like 2

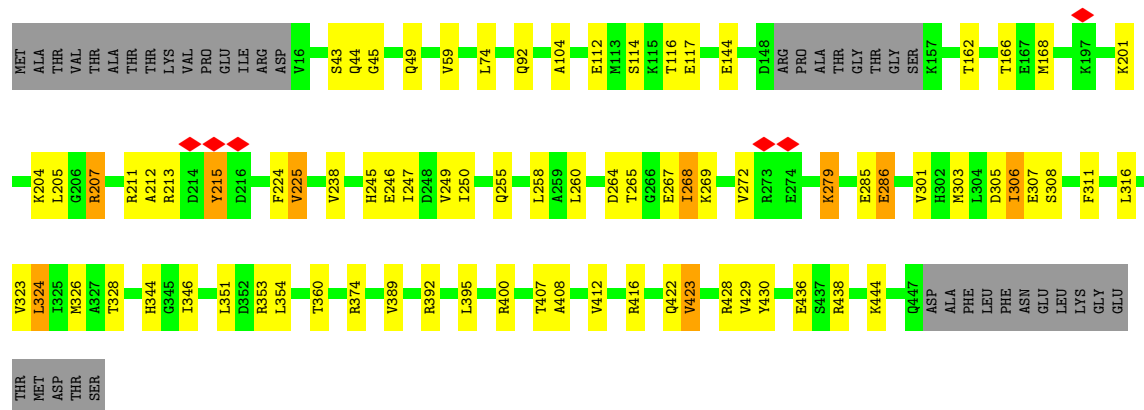
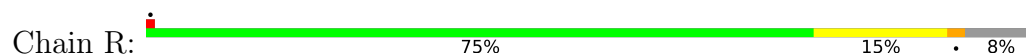


• Molecule 10: RuvB-like 2

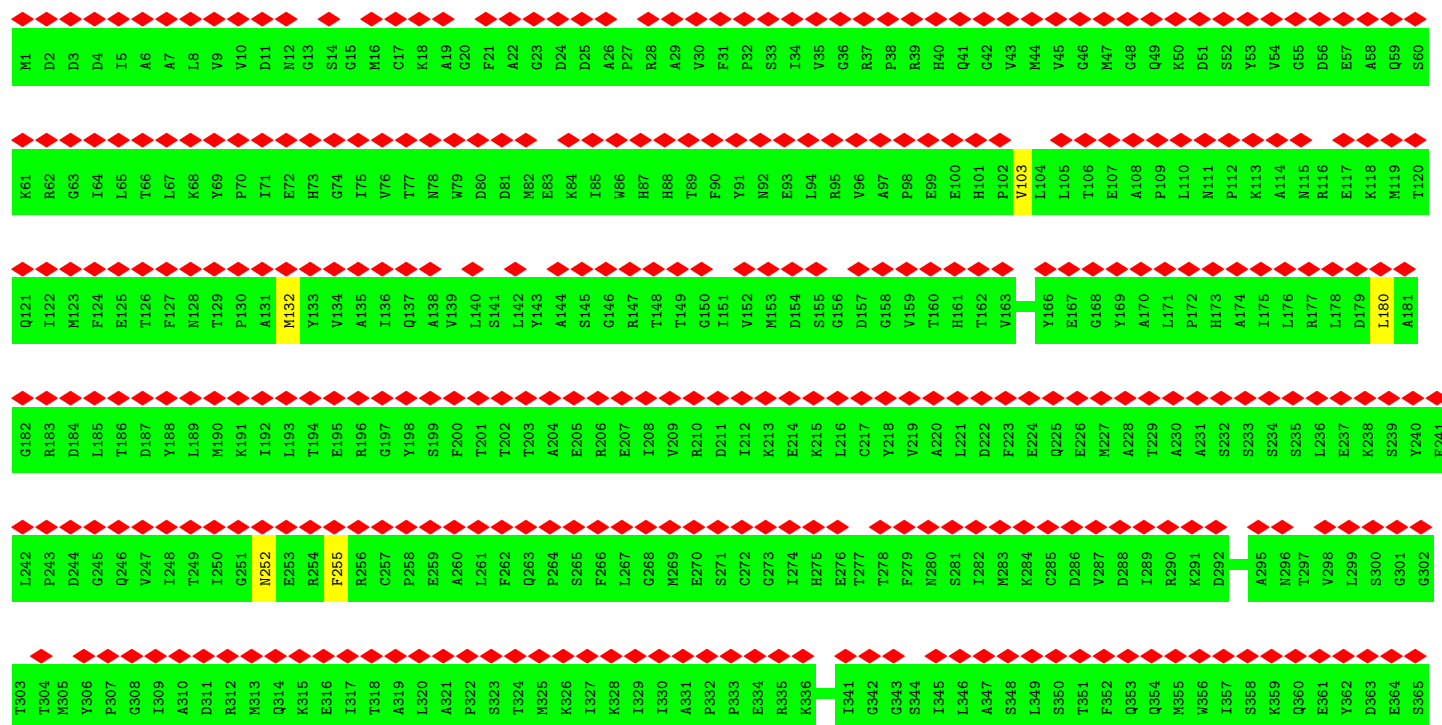


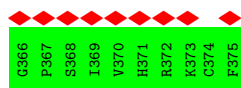


• Molecule 10: RuvB-like 2

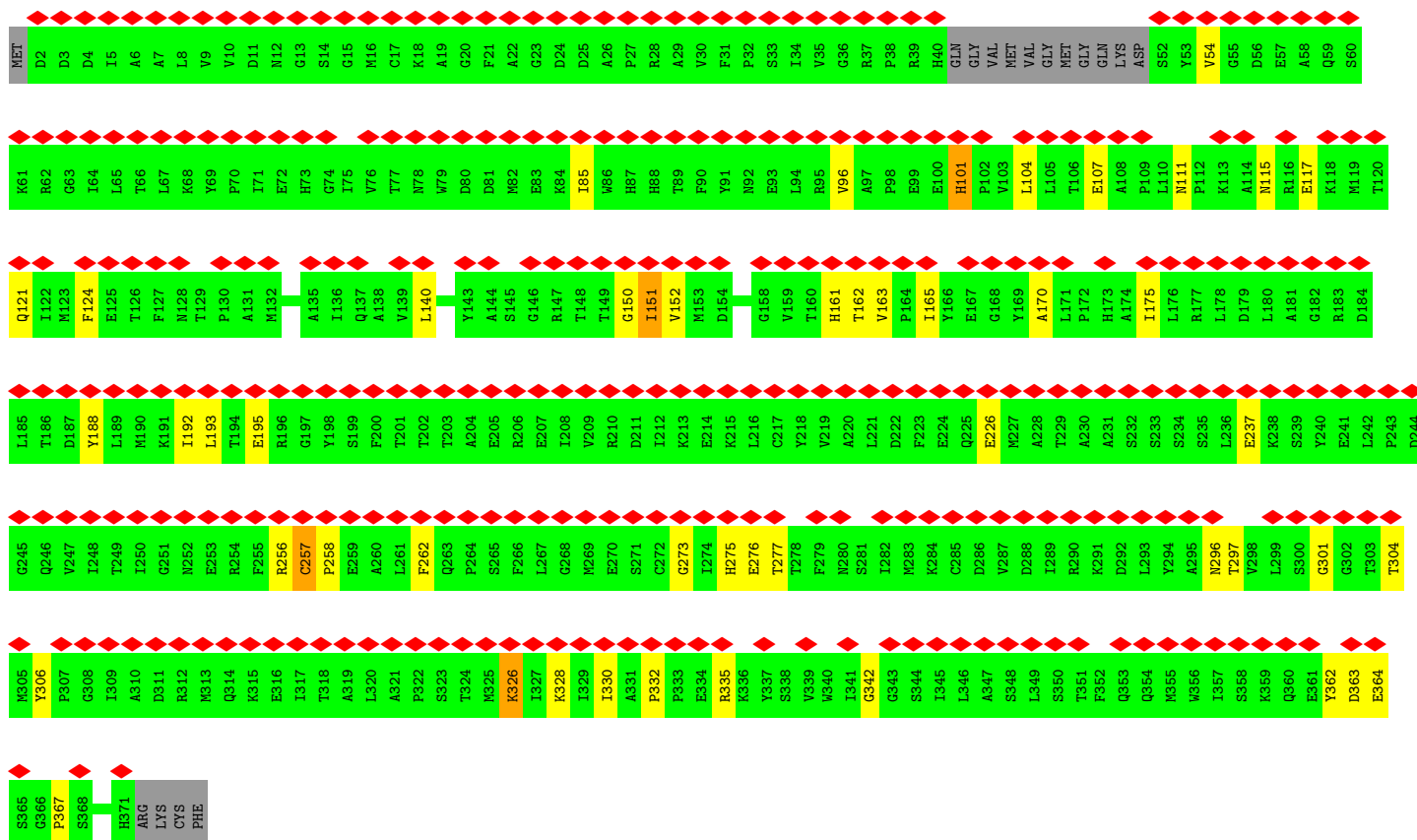
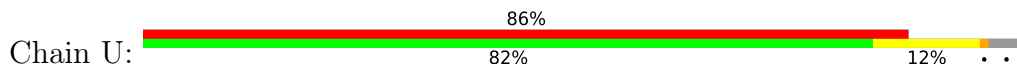


• Molecule 11: Actin, cytoplasmic 1

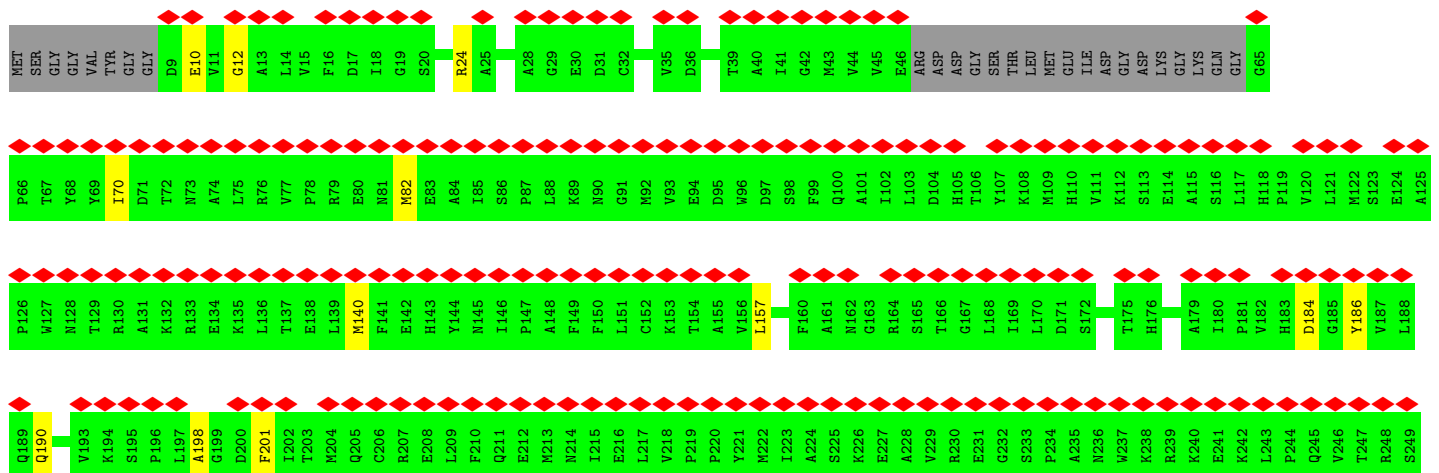
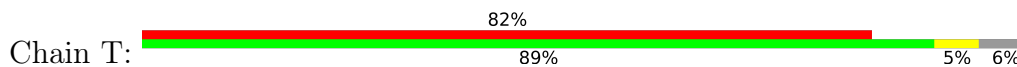


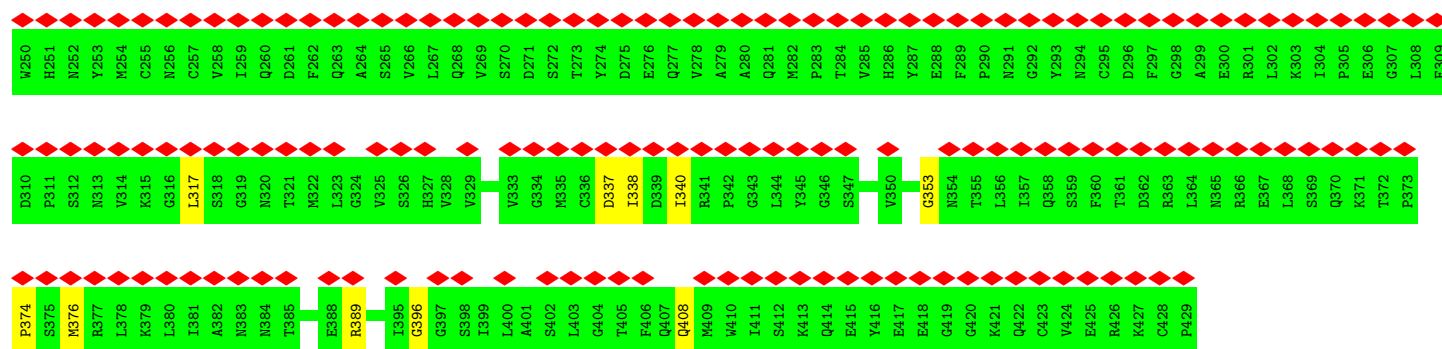


• Molecule 11: Actin, cytoplasmic 1

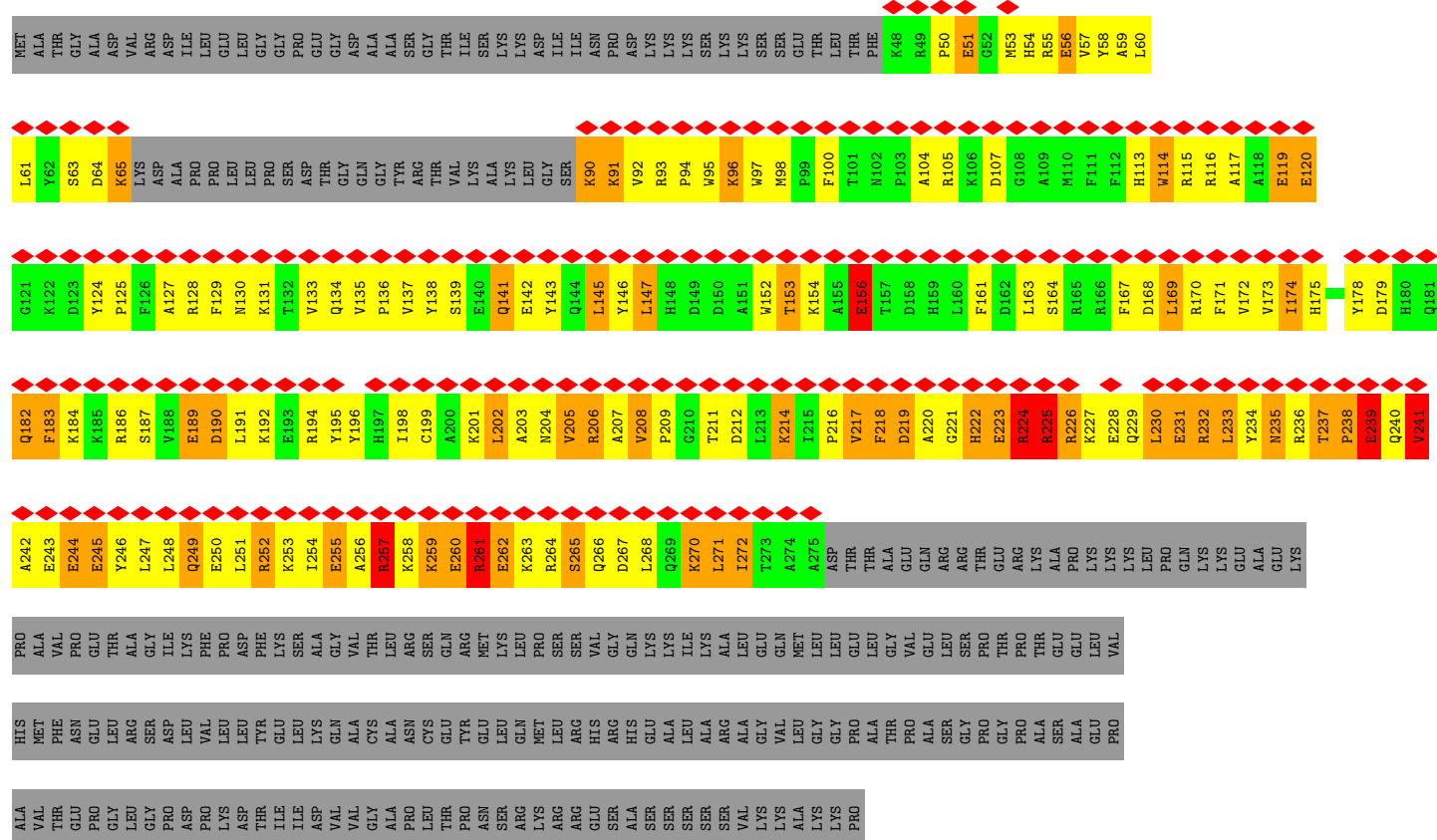
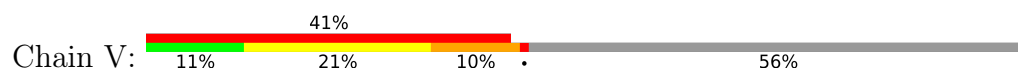


• Molecule 12: Actin-like protein 6A

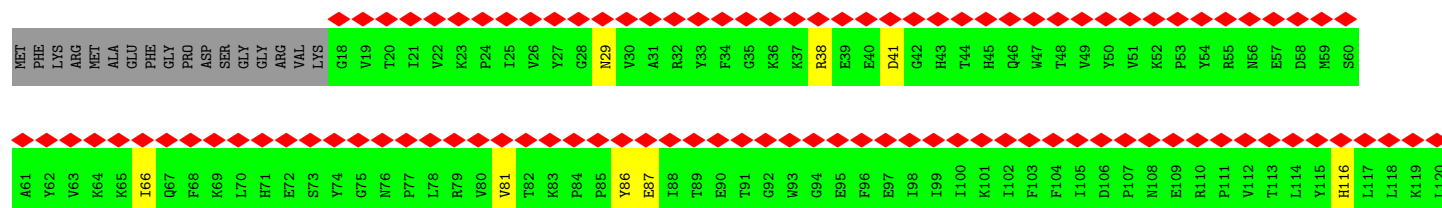
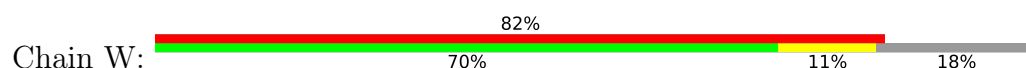


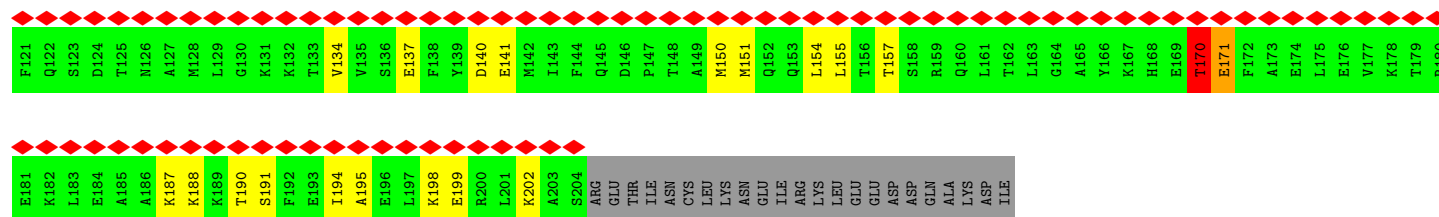


• Molecule 13: DNA methyltransferase 1-associated protein 1

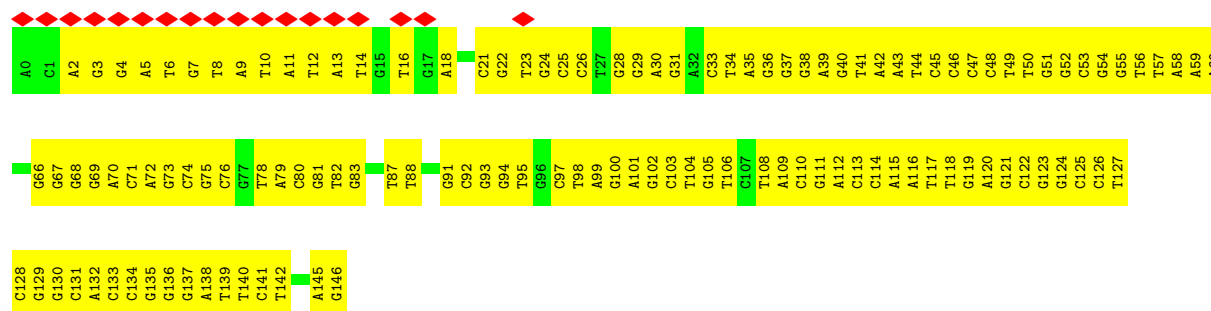


• Molecule 14: YEATS domain-containing protein 4

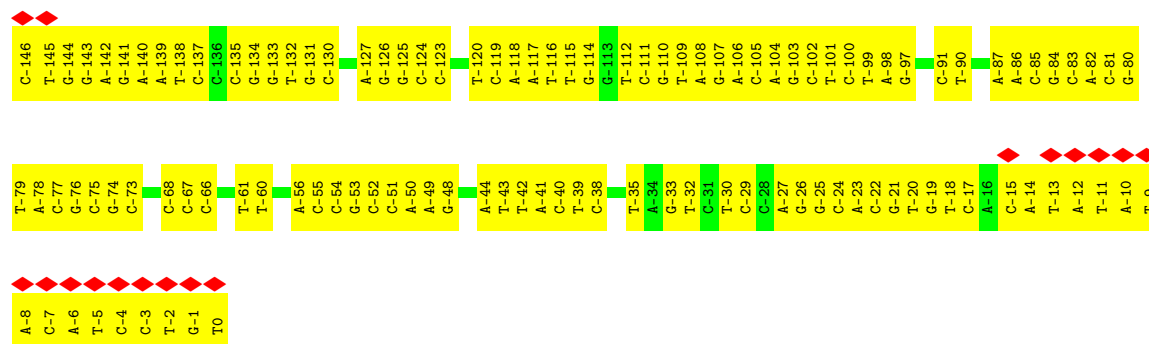




• Molecule 15: DNA (147-MER)



• Molecule 16: DNA (147-MER)



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 475617                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 1500                                    | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.244                                   | Depositor |
| Minimum map value                    | -0.115                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.006                                   | Depositor |
| Recommended contour level            | 0.027                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 533.6, 533.6, 533.6                     | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.334, 1.334, 1.334                     | 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: ADP, MG, ATP, BEF

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     | 0.27         | 0/843          | 0.47        | 0/1136          |
| 1   | E     | 0.18         | 0/818          | 0.47        | 0/1104          |
| 2   | B     | 0.18         | 0/766          | 0.46        | 0/1026          |
| 2   | F     | 0.18         | 0/747          | 0.43        | 0/1004          |
| 3   | C     | 0.18         | 0/789          | 0.45        | 0/1057          |
| 3   | G     | 0.17         | 0/813          | 0.41        | 0/1090          |
| 4   | D     | 0.19         | 0/653          | 0.32        | 0/873           |
| 4   | H     | 0.14         | 0/645          | 0.38        | 0/862           |
| 5   | I     | 0.26         | 1/7296 (0.0%)  | 0.53        | 2/9855 (0.0%)   |
| 6   | J     | 0.32         | 1/1381 (0.1%)  | 0.49        | 0/1861          |
| 7   | K     | 0.26         | 0/3283         | 0.59        | 2/4445 (0.0%)   |
| 8   | L     | 0.41         | 1/909 (0.1%)   | 0.54        | 0/1227          |
| 9   | M     | 0.21         | 0/3253         | 0.51        | 2/4382 (0.0%)   |
| 9   | O     | 0.27         | 0/3382         | 0.55        | 1/4559 (0.0%)   |
| 9   | Q     | 0.21         | 0/3413         | 0.48        | 0/4603          |
| 10  | N     | 0.19         | 0/3217         | 0.48        | 0/4328          |
| 10  | P     | 0.23         | 0/3324         | 0.49        | 0/4477          |
| 10  | R     | 0.21         | 0/3329         | 0.51        | 1/4479 (0.0%)   |
| 11  | S     | 0.18         | 0/2988         | 0.36        | 0/4045          |
| 11  | U     | 0.22         | 0/2863         | 0.48        | 0/3882          |
| 12  | T     | 0.19         | 0/3217         | 0.39        | 0/4362          |
| 13  | V     | 0.46         | 3/1801 (0.2%)  | 0.71        | 8/2419 (0.3%)   |
| 14  | W     | 0.32         | 0/1578         | 0.45        | 0/2128          |
| 15  | X     | 0.22         | 0/3405         | 0.45        | 0/5259          |
| 16  | Y     | 0.21         | 0/3349         | 0.41        | 0/5162          |
| All | All   | 0.24         | 6/58062 (0.0%) | 0.49        | 16/79625 (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 |
|-----|-------|---------------------|---------------------|
| 3   | G     | 0                   | 1                   |
| 5   | I     | 0                   | 1                   |
| 9   | M     | 0                   | 1                   |
| 10  | P     | 0                   | 2                   |
| 10  | R     | 0                   | 1                   |
| 13  | V     | 0                   | 3                   |
| 14  | W     | 0                   | 1                   |
| All | All   | 0                   | 10                  |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 8   | L     | 12  | ASP  | C-O     | -9.54 | 1.19        | 1.23     |
| 5   | I     | 124 | LEU  | C-O     | -6.32 | 1.20        | 1.23     |
| 6   | J     | 165 | ARG  | C-O     | 5.87  | 1.31        | 1.24     |
| 13  | V     | 183 | PHE  | CD1-CE1 | 5.65  | 1.55        | 1.38     |
| 13  | V     | 261 | ARG  | CA-C    | 5.61  | 1.56        | 1.52     |
| 13  | V     | 156 | GLU  | CD-OE1  | 5.06  | 1.34        | 1.25     |

All (16) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 5   | I     | 1995 | PRO  | N-CA-C    | 9.67  | 122.49      | 110.70   |
| 10  | R     | 215  | TYR  | N-CA-C    | -9.66 | 100.59      | 111.71   |
| 13  | V     | 156  | GLU  | CB-CG-CD  | 8.66  | 127.33      | 112.60   |
| 9   | M     | 317  | ARG  | N-CA-C    | -7.92 | 103.75      | 113.50   |
| 13  | V     | 260  | GLU  | CA-C-N    | -6.74 | 114.42      | 122.44   |
| 13  | V     | 260  | GLU  | C-N-CA    | -6.74 | 114.42      | 122.44   |
| 7   | K     | 119  | PHE  | N-CA-C    | 6.61  | 118.84      | 107.28   |
| 7   | K     | 81   | LYS  | N-CA-C    | -6.29 | 106.83      | 114.75   |
| 13  | V     | 224  | ARG  | N-CA-C    | -6.07 | 104.57      | 111.07   |
| 13  | V     | 261  | ARG  | O-C-N     | -5.96 | 114.90      | 121.76   |
| 9   | M     | 192  | TYR  | CB-CA-C   | 5.70  | 120.23      | 111.85   |
| 5   | I     | 1995 | PRO  | CB-CA-C   | -5.58 | 104.12      | 110.92   |
| 13  | V     | 262  | GLU  | CA-CB-CG  | -5.55 | 102.99      | 114.10   |
| 13  | V     | 241  | VAL  | N-CA-C    | -5.46 | 107.11      | 111.81   |
| 9   | O     | 18   | HIS  | N-CA-C    | -5.43 | 104.91      | 112.30   |
| 13  | V     | 156  | GLU  | CG-CD-OE2 | -5.39 | 106.01      | 118.40   |

There are no chirality outliers.

All (10) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 3   | G     | 134  | ARG  | Sidechain |
| 5   | I     | 2029 | ARG  | Sidechain |
| 9   | M     | 317  | ARG  | Sidechain |
| 10  | P     | 18   | ARG  | Sidechain |
| 10  | P     | 21   | ARG  | Sidechain |
| 10  | R     | 213  | ARG  | Sidechain |
| 13  | V     | 225  | ARG  | Sidechain |
| 13  | V     | 257  | ARG  | Sidechain |
| 13  | V     | 261  | ARG  | Mainchain |
| 14  | W     | 170  | THR  | Peptide   |

## 5.2 Too-close contacts [i](#)

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     | 833   | 0        | 895      | 188     | 0            |
| 1   | E     | 808   | 0        | 864      | 118     | 0            |
| 2   | B     | 755   | 0        | 782      | 139     | 0            |
| 2   | F     | 736   | 0        | 756      | 69      | 0            |
| 3   | C     | 779   | 0        | 816      | 75      | 0            |
| 3   | G     | 801   | 0        | 839      | 95      | 0            |
| 4   | D     | 646   | 0        | 687      | 37      | 0            |
| 4   | H     | 638   | 0        | 676      | 63      | 0            |
| 5   | I     | 7122  | 0        | 7212     | 322     | 0            |
| 6   | J     | 1350  | 0        | 1370     | 28      | 0            |
| 7   | K     | 3209  | 0        | 3132     | 549     | 0            |
| 8   | L     | 893   | 0        | 880      | 55      | 0            |
| 9   | M     | 3213  | 0        | 3331     | 94      | 0            |
| 9   | O     | 3339  | 0        | 3425     | 31      | 0            |
| 9   | Q     | 3368  | 0        | 3453     | 33      | 0            |
| 10  | N     | 3185  | 0        | 3269     | 47      | 0            |
| 10  | P     | 3287  | 0        | 3335     | 24      | 0            |
| 10  | R     | 3293  | 0        | 3373     | 47      | 0            |
| 11  | S     | 2925  | 0        | 2891     | 2       | 0            |
| 11  | U     | 2802  | 0        | 2760     | 34      | 0            |
| 12  | T     | 3146  | 0        | 3086     | 21      | 0            |
| 13  | V     | 1757  | 0        | 1736     | 330     | 0            |
| 14  | W     | 1542  | 0        | 1556     | 70      | 0            |
| 15  | X     | 3031  | 0        | 1650     | 242     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16  | Y     | 2990  | 0        | 1652     | 181     | 0            |
| 17  | I     | 27    | 0        | 12       | 6       | 0            |
| 17  | M     | 27    | 0        | 12       | 0       | 0            |
| 17  | N     | 27    | 0        | 12       | 0       | 0            |
| 17  | O     | 27    | 0        | 12       | 1       | 0            |
| 17  | P     | 27    | 0        | 12       | 0       | 0            |
| 17  | Q     | 27    | 0        | 12       | 0       | 0            |
| 17  | R     | 27    | 0        | 12       | 0       | 0            |
| 18  | I     | 1     | 0        | 0        | 0       | 0            |
| 19  | I     | 4     | 0        | 0        | 3       | 0            |
| 20  | T     | 31    | 0        | 12       | 1       | 0            |
| 20  | U     | 31    | 0        | 12       | 0       | 0            |
| All | All   | 56704 | 0        | 54534    | 2341    | 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 21.

All (2341) 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) |
|-------------------|------------------|--------------------------|-------------------|
| 9:M:313:THR:HA    | 9:M:316:HIS:CE1  | 1.28                     | 1.63              |
| 1:A:13:ALA:HB2    | 5:I:164:LYS:CD   | 1.25                     | 1.61              |
| 9:M:413:ALA:HA    | 9:M:433:ILE:CD1  | 1.35                     | 1.53              |
| 5:I:936:HIS:CE1   | 10:N:279:LYS:HZ3 | 1.29                     | 1.48              |
| 5:I:936:HIS:HE1   | 10:N:279:LYS:NZ  | 1.08                     | 1.47              |
| 5:I:2063:LEU:HD21 | 5:I:2127:LEU:CD2 | 1.44                     | 1.46              |
| 5:I:732:HIS:HD2   | 5:I:736:ARG:NH1  | 1.17                     | 1.41              |
| 5:I:2014:LEU:HD12 | 9:Q:259:MET:SD   | 1.62                     | 1.39              |
| 6:J:269:SER:HB2   | 9:Q:150:TYR:CD1  | 1.55                     | 1.39              |
| 5:I:936:HIS:CE1   | 10:N:279:LYS:NZ  | 1.87                     | 1.35              |
| 5:I:732:HIS:CD2   | 5:I:736:ARG:HH12 | 1.45                     | 1.33              |
| 1:A:13:ALA:CB     | 5:I:164:LYS:HD2  | 1.60                     | 1.31              |
| 5:I:921:ILE:CG2   | 5:I:1986:PRO:HD2 | 1.62                     | 1.28              |
| 1:A:13:ALA:CB     | 5:I:164:LYS:CD   | 2.14                     | 1.25              |
| 5:I:969:LEU:HD22  | 10:R:224:PHE:O   | 1.31                     | 1.25              |
| 5:I:921:ILE:HG21  | 5:I:1986:PRO:CD  | 1.66                     | 1.24              |
| 5:I:949:ILE:HG21  | 9:M:247:ASN:O    | 1.11                     | 1.23              |
| 9:M:26:LEU:HD22   | 9:M:30:GLY:O     | 1.37                     | 1.23              |
| 5:I:949:ILE:CG2   | 9:M:247:ASN:O    | 1.87                     | 1.22              |
| 9:M:313:THR:CA    | 9:M:316:HIS:CE1  | 2.21                     | 1.22              |
| 6:J:269:SER:HB2   | 9:Q:150:TYR:CG   | 1.73                     | 1.22              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:J:269:SER:CB    | 9:Q:150:TYR:HB3   | 1.73                     | 1.19              |
| 5:I:1983:VAL:CG2  | 9:O:238:VAL:HG11  | 1.76                     | 1.16              |
| 1:E:20:ARG:CG     | 2:F:121:SER:OG    | 1.92                     | 1.16              |
| 5:I:1972:ILE:HG23 | 5:I:1976:PHE:CD2  | 1.80                     | 1.15              |
| 5:I:2063:LEU:HD21 | 5:I:2127:LEU:HD21 | 1.27                     | 1.15              |
| 9:M:413:ALA:CA    | 9:M:433:ILE:CD1   | 2.26                     | 1.15              |
| 5:I:660:LEU:HD23  | 5:I:742:TYR:CZ    | 1.82                     | 1.14              |
| 5:I:2014:LEU:CD1  | 9:Q:259:MET:SD    | 2.34                     | 1.14              |
| 5:I:2060:HIS:NE2  | 5:I:2132:THR:HG21 | 1.59                     | 1.14              |
| 8:L:27:ARG:HE     | 8:L:153:THR:CG2   | 1.61                     | 1.13              |
| 9:O:34:GLN:OE1    | 9:O:43:GLU:OE2    | 1.65                     | 1.12              |
| 5:I:732:HIS:CD2   | 5:I:736:ARG:NH1   | 2.10                     | 1.12              |
| 5:I:667:TRP:NE1   | 5:I:719:HIS:ND1   | 1.98                     | 1.11              |
| 6:J:269:SER:CA    | 9:Q:150:TYR:HB3   | 1.81                     | 1.11              |
| 13:V:239:GLU:HA   | 13:V:243:GLU:HB2  | 1.33                     | 1.11              |
| 5:I:921:ILE:HG22  | 5:I:1985:ALA:HB1  | 1.29                     | 1.11              |
| 9:M:113:MET:HG3   | 9:M:276:ARG:NH1   | 1.65                     | 1.10              |
| 1:E:67:GLY:HA2    | 1:E:78:ILE:HG12   | 1.32                     | 1.10              |
| 8:L:27:ARG:HE     | 8:L:153:THR:HG22  | 1.17                     | 1.10              |
| 13:V:136:PRO:HB2  | 13:V:202:LEU:HD12 | 1.31                     | 1.09              |
| 5:I:969:LEU:CD2   | 10:R:224:PHE:O    | 2.01                     | 1.08              |
| 15:X:22:DG:H2"    | 15:X:23:DT:H5"    | 1.23                     | 1.08              |
| 5:I:2060:HIS:NE2  | 5:I:2132:THR:CG2  | 2.14                     | 1.08              |
| 16:Y:-140:DA:H2"  | 16:Y:-139:DA:H5"  | 1.36                     | 1.07              |
| 5:I:667:TRP:HE1   | 5:I:719:HIS:CE1   | 1.72                     | 1.06              |
| 5:I:810:PRO:O     | 5:I:814:MET:HG2   | 1.53                     | 1.06              |
| 9:M:413:ALA:HA    | 9:M:433:ILE:HD12  | 1.32                     | 1.06              |
| 6:J:269:SER:CB    | 9:Q:150:TYR:CB    | 2.34                     | 1.06              |
| 7:K:56:TYR:HB2    | 8:L:39:ASN:ND2    | 1.70                     | 1.06              |
| 13:V:153:THR:HG23 | 13:V:156:GLU:HB2  | 1.36                     | 1.05              |
| 5:I:667:TRP:NE1   | 5:I:719:HIS:CE1   | 2.24                     | 1.05              |
| 1:A:13:ALA:HB2    | 5:I:164:LYS:HD2   | 1.07                     | 1.05              |
| 5:I:670:HIS:NE2   | 5:I:742:TYR:HD2   | 1.53                     | 1.05              |
| 9:M:413:ALA:HA    | 9:M:433:ILE:HD13  | 1.36                     | 1.04              |
| 9:M:110:GLU:OE2   | 9:M:276:ARG:NH2   | 1.89                     | 1.04              |
| 8:L:27:ARG:NE     | 8:L:153:THR:HG22  | 1.73                     | 1.03              |
| 5:I:621:TYR:CE2   | 5:I:846:GLU:OE1   | 2.11                     | 1.03              |
| 13:V:96:LYS:HD2   | 13:V:98:MET:HG2   | 1.38                     | 1.02              |
| 5:I:949:ILE:HG22  | 10:R:260:LEU:HD22 | 1.36                     | 1.02              |
| 5:I:163:ARG:O     | 5:I:166:VAL:HG22  | 1.58                     | 1.02              |
| 7:K:6:LEU:HD12    | 7:K:93:ILE:HD11   | 1.41                     | 1.02              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:J:269:SER:CB    | 9:Q:150:TYR:CG    | 2.42                     | 1.02              |
| 1:E:20:ARG:HG3    | 2:F:121:SER:OG    | 1.59                     | 1.01              |
| 5:I:921:ILE:HD13  | 5:I:1986:PRO:HG2  | 1.38                     | 1.01              |
| 5:I:2063:LEU:HD21 | 5:I:2127:LEU:HD23 | 1.40                     | 1.01              |
| 5:I:2063:LEU:CD2  | 5:I:2127:LEU:CD2  | 2.39                     | 1.00              |
| 9:M:313:THR:HA    | 9:M:316:HIS:ND1   | 1.76                     | 1.00              |
| 13:V:264:ARG:HH12 | 14:W:194:ILE:HD13 | 1.23                     | 0.99              |
| 7:K:81:LYS:HA     | 7:K:85:GLN:HA     | 1.42                     | 0.99              |
| 13:V:233:LEU:HA   | 13:V:236:ARG:HD3  | 1.38                     | 0.99              |
| 5:I:660:LEU:HD23  | 5:I:742:TYR:OH    | 1.62                     | 0.99              |
| 5:I:660:LEU:CD2   | 5:I:742:TYR:OH    | 2.10                     | 0.99              |
| 5:I:901:CYS:O     | 5:I:2044:LYS:CE   | 2.11                     | 0.99              |
| 5:I:670:HIS:CE1   | 5:I:742:TYR:CD2   | 2.51                     | 0.99              |
| 1:A:13:ALA:HB2    | 5:I:164:LYS:HD3   | 1.02                     | 0.98              |
| 5:I:670:HIS:NE2   | 5:I:742:TYR:CD2   | 2.31                     | 0.98              |
| 6:J:269:SER:HA    | 9:Q:150:TYR:HB3   | 1.40                     | 0.98              |
| 7:K:233:MET:HA    | 7:K:255:MET:HE1   | 1.46                     | 0.98              |
| 7:K:56:TYR:CB     | 8:L:39:ASN:HD21   | 1.75                     | 0.98              |
| 15:X:48:DC:H2''   | 15:X:49:DT:H71    | 1.45                     | 0.98              |
| 7:K:146:ILE:HD11  | 7:K:317:ILE:HG12  | 1.44                     | 0.97              |
| 1:A:59:LEU:HD11   | 2:B:66:ILE:HG21   | 1.44                     | 0.97              |
| 4:D:23:ARG:HH21   | 14:W:81:VAL:HG11  | 1.28                     | 0.97              |
| 5:I:2087:LEU:HD11 | 5:I:2104:ARG:NH1  | 1.79                     | 0.97              |
| 3:C:127:ALA:HA    | 3:G:130:ILE:HD13  | 1.42                     | 0.97              |
| 9:M:413:ALA:HA    | 9:M:433:ILE:HD11  | 1.45                     | 0.96              |
| 13:V:237:THR:HG23 | 13:V:238:PRO:HD3  | 1.46                     | 0.96              |
| 5:I:2072:LEU:HB3  | 5:I:2088:ARG:HD2  | 1.45                     | 0.96              |
| 11:U:121:GLN:NE2  | 13:V:95:TRP:O     | 1.98                     | 0.96              |
| 9:M:110:GLU:HG2   | 9:M:269:THR:HG22  | 1.48                     | 0.96              |
| 10:N:38:GLU:OE1   | 10:N:54:ARG:NH1   | 1.98                     | 0.96              |
| 15:X:51:DG:H1'    | 15:X:52:DG:H5'    | 1.46                     | 0.96              |
| 6:J:269:SER:CB    | 9:Q:150:TYR:CD1   | 2.48                     | 0.95              |
| 16:Y:-50:DA:H2''  | 16:Y:-49:DA:H5''  | 1.48                     | 0.95              |
| 9:M:313:THR:HA    | 9:M:316:HIS:HE1   | 1.17                     | 0.94              |
| 16:Y:-14:DA:H2''  | 16:Y:-13:DT:C7    | 1.97                     | 0.94              |
| 3:G:73:GLU:HA     | 4:H:23:ARG:HH22   | 1.32                     | 0.94              |
| 10:N:73:VAL:HB    | 10:N:325:ILE:HG12 | 1.50                     | 0.94              |
| 13:V:264:ARG:HB3  | 14:W:198:LYS:CE   | 1.95                     | 0.94              |
| 16:Y:-52:DC:H1'   | 16:Y:-51:DC:H5'   | 1.47                     | 0.94              |
| 2:F:29:SER:HB3    | 16:Y:-119:DC:H4'  | 1.47                     | 0.94              |
| 10:N:324:LEU:CD1  | 10:N:326:MET:HE3  | 1.96                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:I:163:ARG:O     | 5:I:166:VAL:CG2   | 2.15                     | 0.93              |
| 13:V:264:ARG:HB3  | 14:W:198:LYS:HE2  | 1.47                     | 0.93              |
| 16:Y:-145:DT:H2'' | 16:Y:-144:DG:H5'' | 1.46                     | 0.93              |
| 7:K:234:ILE:HD12  | 7:K:271:ALA:HA    | 1.47                     | 0.93              |
| 15:X:73:DG:O6     | 16:Y:-73:DC:N4    | 2.01                     | 0.93              |
| 1:A:21:ARG:HH11   | 1:A:21:ARG:HB2    | 1.30                     | 0.93              |
| 1:A:59:LEU:HB2    | 2:B:62:PHE:HZ     | 1.30                     | 0.93              |
| 5:I:921:ILE:HD13  | 5:I:1986:PRO:CG   | 1.98                     | 0.93              |
| 9:M:193:ILE:HG12  | 9:M:200:VAL:HG22  | 1.49                     | 0.93              |
| 5:I:2120:SER:OG   | 15:X:55:DG:O5'    | 1.85                     | 0.92              |
| 13:V:98:MET:SD    | 13:V:115:ARG:HB2  | 2.09                     | 0.92              |
| 7:K:128:GLY:HA2   | 7:K:147:ILE:HG21  | 1.48                     | 0.92              |
| 4:D:23:ARG:HH21   | 14:W:81:VAL:CG1   | 1.82                     | 0.92              |
| 5:I:1972:ILE:HG23 | 5:I:1976:PHE:HD2  | 1.24                     | 0.92              |
| 5:I:936:HIS:HE1   | 10:N:279:LYS:HZ1  | 0.95                     | 0.92              |
| 5:I:921:ILE:HG21  | 5:I:1986:PRO:HD2  | 0.92                     | 0.91              |
| 4:D:75:HIS:O      | 2:F:89:ARG:NH1    | 2.03                     | 0.90              |
| 5:I:667:TRP:NE1   | 5:I:719:HIS:HD1   | 1.64                     | 0.90              |
| 15:X:48:DC:H2''   | 15:X:49:DT:C7     | 2.01                     | 0.90              |
| 7:K:56:TYR:O      | 8:L:39:ASN:ND2    | 2.03                     | 0.90              |
| 7:K:165:LYS:HG2   | 7:K:167:LYS:HD2   | 1.52                     | 0.90              |
| 1:A:116:LEU:HD11  | 3:C:108:ASN:HD21  | 1.35                     | 0.90              |
| 5:I:901:CYS:O     | 5:I:2044:LYS:HE2  | 1.71                     | 0.90              |
| 13:V:261:ARG:HD2  | 14:W:198:LYS:CG   | 2.01                     | 0.90              |
| 16:Y:-116:DT:C6   | 16:Y:-115:DT:H72  | 2.06                     | 0.90              |
| 6:J:162:HIS:CE1   | 15:X:137:DG:H4'   | 2.07                     | 0.90              |
| 16:Y:-131:DG:H2'' | 16:Y:-130:DC:C5   | 2.06                     | 0.90              |
| 3:G:79:LYS:HG2    | 3:G:82:LEU:HG     | 1.53                     | 0.90              |
| 13:V:96:LYS:HB3   | 13:V:98:MET:HE3   | 1.53                     | 0.89              |
| 13:V:250:GLU:O    | 13:V:254:ILE:HG23 | 1.72                     | 0.89              |
| 1:E:102:ILE:HG23  | 2:F:58:ILE:HD13   | 1.53                     | 0.89              |
| 15:X:3:DG:H2''    | 15:X:4:DG:H5'     | 1.52                     | 0.89              |
| 15:X:136:DG:H5''  | 15:X:136:DG:H8    | 1.35                     | 0.89              |
| 1:E:64:GLU:HB2    | 2:F:45:VAL:HG11   | 1.54                     | 0.89              |
| 9:M:125:LYS:HG2   | 9:M:235:ILE:HG12  | 1.54                     | 0.89              |
| 5:I:2044:LYS:NZ   | 5:I:2173:GLU:OE1  | 2.04                     | 0.89              |
| 16:Y:-102:DC:H2'' | 16:Y:-101:DT:H72  | 1.55                     | 0.89              |
| 1:A:25:GLN:NE2    | 8:L:7:SER:O       | 2.06                     | 0.89              |
| 5:I:713:THR:OG1   | 15:X:135:DG:O3'   | 1.89                     | 0.89              |
| 16:Y:-5:DT:H2''   | 16:Y:-4:DC:H5'    | 1.52                     | 0.89              |
| 7:K:56:TYR:CB     | 8:L:39:ASN:ND2    | 2.35                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:I:667:TRP:CD1   | 5:I:719:HIS:HD1   | 1.92                     | 0.88              |
| 1:A:59:LEU:CD1    | 2:B:66:ILE:HG21   | 2.04                     | 0.88              |
| 5:I:660:LEU:CD2   | 5:I:742:TYR:CZ    | 2.56                     | 0.88              |
| 1:A:82:ARG:HB2    | 3:C:58:THR:HG21   | 1.54                     | 0.88              |
| 1:A:42:GLU:HG2    | 2:B:84:SER:HB2    | 1.56                     | 0.88              |
| 7:K:211:TYR:HE1   | 7:K:274:ARG:HD3   | 1.36                     | 0.88              |
| 3:C:109:LEU:HD13  | 3:G:129:ARG:HG2   | 1.54                     | 0.88              |
| 13:V:187:SER:OG   | 13:V:190:ASP:OD1  | 1.91                     | 0.87              |
| 1:A:23:GLY:O      | 8:L:9:ARG:NH1     | 2.08                     | 0.87              |
| 1:A:82:ARG:NH2    | 1:A:108:VAL:O     | 2.06                     | 0.87              |
| 5:I:621:TYR:HE2   | 5:I:846:GLU:OE1   | 1.53                     | 0.87              |
| 7:K:106:GLN:HB3   | 7:K:124:ARG:HH22  | 1.40                     | 0.87              |
| 7:K:106:GLN:HB3   | 7:K:124:ARG:NH2   | 1.90                     | 0.87              |
| 15:X:48:DC:OP2    | 15:X:48:DC:H2'    | 1.75                     | 0.87              |
| 1:E:63:LEU:HD13   | 2:F:42:LEU:HB2    | 1.56                     | 0.86              |
| 7:K:236:TYR:HB3   | 7:K:269:ARG:HG3   | 1.57                     | 0.86              |
| 13:V:164:SER:HA   | 13:V:174:ILE:HD11 | 1.56                     | 0.86              |
| 5:I:2014:LEU:HG   | 5:I:2017:ARG:HD2  | 1.57                     | 0.86              |
| 16:Y:-21:DG:H2'   | 16:Y:-20:DT:H71   | 1.57                     | 0.86              |
| 15:X:22:DG:C2'    | 15:X:23:DT:H5''   | 2.05                     | 0.86              |
| 7:K:5:VAL:HA      | 7:K:94:ILE:HG23   | 1.55                     | 0.86              |
| 7:K:26:PRO:HG2    | 7:K:42:ALA:HA     | 1.56                     | 0.86              |
| 15:X:45:DC:H2''   | 15:X:46:DC:H5''   | 1.58                     | 0.85              |
| 5:I:657:LEU:CD2   | 5:I:670:HIS:ND1   | 2.40                     | 0.85              |
| 5:I:2037:LEU:CD1  | 5:I:2039:GLN:HG2  | 2.06                     | 0.85              |
| 1:A:59:LEU:HB2    | 2:B:62:PHE:CZ     | 2.10                     | 0.85              |
| 6:J:269:SER:HB2   | 9:Q:150:TYR:CB    | 1.99                     | 0.85              |
| 5:I:1983:VAL:HG23 | 9:O:238:VAL:HG11  | 1.58                     | 0.85              |
| 9:M:113:MET:HG3   | 9:M:276:ARG:HH12  | 1.37                     | 0.85              |
| 3:C:110:CYS:SG    | 3:G:130:ILE:HD11  | 2.16                     | 0.85              |
| 13:V:261:ARG:HD2  | 14:W:198:LYS:HG3  | 1.56                     | 0.85              |
| 1:E:57:TYR:HA     | 6:J:130:ARG:HH12  | 1.40                     | 0.85              |
| 1:E:106:GLY:HA3   | 3:G:58:THR:HG22   | 1.59                     | 0.85              |
| 7:K:146:ILE:HG22  | 7:K:158:VAL:H     | 1.41                     | 0.85              |
| 6:J:269:SER:HB2   | 9:Q:150:TYR:HD1   | 1.42                     | 0.85              |
| 9:M:413:ALA:CA    | 9:M:433:ILE:HD12  | 2.02                     | 0.85              |
| 5:I:2060:HIS:CD2  | 5:I:2132:THR:HG23 | 2.12                     | 0.84              |
| 16:Y:-146:DC:H6   | 16:Y:-146:DC:H5'  | 1.42                     | 0.84              |
| 15:X:116:DA:H2''  | 15:X:117:DT:H5'   | 1.59                     | 0.84              |
| 13:V:264:ARG:HG2  | 13:V:264:ARG:HH11 | 1.41                     | 0.84              |
| 10:N:324:LEU:HD13 | 10:N:326:MET:HE3  | 1.58                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:K:56:TYR:HB2    | 8:L:39:ASN:HD21   | 1.35                     | 0.83              |
| 9:O:34:GLN:CD     | 9:O:43:GLU:OE2    | 2.20                     | 0.83              |
| 9:M:26:LEU:HD11   | 9:M:50:GLY:HA3    | 1.58                     | 0.83              |
| 4:D:92:ARG:NH2    | 2:F:97:LEU:O      | 2.12                     | 0.83              |
| 16:Y:-14:DA:H2''  | 16:Y:-13:DT:H73   | 1.59                     | 0.83              |
| 16:Y:-125:DG:H2'' | 16:Y:-124:DC:H5'' | 1.60                     | 0.83              |
| 13:V:244:GLU:O    | 13:V:247:LEU:HG   | 1.77                     | 0.83              |
| 13:V:116:ARG:N    | 13:V:119:GLU:OE2  | 2.12                     | 0.83              |
| 4:D:23:ARG:NH2    | 14:W:87:GLU:O     | 2.12                     | 0.82              |
| 9:M:413:ALA:CA    | 9:M:433:ILE:HD13  | 2.00                     | 0.82              |
| 13:V:156:GLU:OE1  | 13:V:183:PHE:CG   | 2.31                     | 0.82              |
| 15:X:73:DG:N1     | 16:Y:-73:DC:N3    | 2.27                     | 0.82              |
| 1:A:32:HIS:O      | 1:A:36:ARG:HG2    | 1.80                     | 0.82              |
| 7:K:196:MET:O     | 8:L:41:GLN:NE2    | 2.13                     | 0.81              |
| 1:E:92:GLU:HG3    | 2:F:100:PRO:HB2   | 1.62                     | 0.81              |
| 5:I:2060:HIS:HD2  | 5:I:2131:ASP:OD2  | 1.63                     | 0.81              |
| 15:X:2:DA:H2''    | 15:X:3:DG:N7      | 1.96                     | 0.81              |
| 1:A:89:ARG:HB2    | 1:A:109:LEU:HD21  | 1.60                     | 0.81              |
| 5:I:118:PHE:CE1   | 13:V:247:LEU:HD22 | 2.16                     | 0.81              |
| 5:I:622:GLN:OE1   | 17:I:3301:ADP:N6  | 2.12                     | 0.81              |
| 10:N:231:GLU:HB2  | 10:N:234:LYS:CE   | 2.10                     | 0.81              |
| 15:X:43:DA:H2''   | 15:X:44:DT:H5''   | 1.60                     | 0.81              |
| 2:B:28:ARG:NE     | 2:B:28:ARG:HA     | 1.96                     | 0.81              |
| 13:V:201:LYS:HD2  | 13:V:204:ASN:HD22 | 1.45                     | 0.81              |
| 1:A:27:PRO:HD3    | 2:B:37:TYR:CD2    | 2.15                     | 0.81              |
| 3:G:106:ASP:HB3   | 3:G:127:ALA:HB1   | 1.63                     | 0.80              |
| 15:X:46:DC:H4'    | 15:X:46:DC:OP1    | 1.77                     | 0.80              |
| 3:C:65:LEU:HB2    | 15:X:91:DG:OP2    | 1.80                     | 0.80              |
| 10:N:301:VAL:HG21 | 10:N:326:MET:HB2  | 1.61                     | 0.80              |
| 16:Y:-82:DA:H1'   | 16:Y:-81:DC:H5'   | 1.62                     | 0.80              |
| 3:G:106:ASP:OD2   | 3:G:131:ARG:NE    | 2.12                     | 0.80              |
| 5:I:949:ILE:HD12  | 9:M:249:ARG:O     | 1.82                     | 0.80              |
| 8:L:27:ARG:NE     | 8:L:153:THR:CG2   | 2.37                     | 0.80              |
| 13:V:136:PRO:HB2  | 13:V:202:LEU:CD1  | 2.08                     | 0.80              |
| 13:V:264:ARG:NH1  | 14:W:194:ILE:HD13 | 1.96                     | 0.80              |
| 1:A:26:PHE:CD1    | 1:A:57:GLU:HB2    | 2.16                     | 0.80              |
| 7:K:159:PRO:HB2   | 7:K:166:LYS:HB2   | 1.63                     | 0.80              |
| 7:K:139:ASN:HB3   | 7:K:142:GLU:HG2   | 1.62                     | 0.80              |
| 13:V:239:GLU:CA   | 13:V:243:GLU:HB2  | 2.11                     | 0.80              |
| 5:I:2060:HIS:CD2  | 5:I:2132:THR:CG2  | 2.65                     | 0.80              |
| 16:Y:-107:DG:H1'  | 16:Y:-106:DA:C8   | 2.16                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Y:-133:DG:C8   | 16:Y:-132:DT:H72  | 2.17                     | 0.79              |
| 5:I:846:GLU:HG2   | 5:I:848:GLN:HG2   | 1.63                     | 0.79              |
| 5:I:1983:VAL:HG21 | 9:O:238:VAL:HG11  | 1.62                     | 0.79              |
| 5:I:2014:LEU:O    | 5:I:2014:LEU:HD23 | 1.82                     | 0.79              |
| 7:K:352:PRO:HB3   | 7:K:358:TYR:CD1   | 2.18                     | 0.79              |
| 7:K:376:VAL:HG13  | 7:K:377:VAL:N     | 1.96                     | 0.79              |
| 5:I:694:LYS:HB2   | 5:I:719:HIS:CD2   | 2.18                     | 0.79              |
| 7:K:5:VAL:O       | 7:K:15:ILE:HA     | 1.83                     | 0.79              |
| 7:K:379:ARG:HA    | 7:K:382:TYR:HB3   | 1.65                     | 0.79              |
| 6:J:269:SER:HB3   | 9:Q:150:TYR:CB    | 2.12                     | 0.79              |
| 7:K:222:ILE:O     | 7:K:230:ASN:HB2   | 1.82                     | 0.79              |
| 7:K:374:ASP:OD1   | 7:K:374:ASP:N     | 2.15                     | 0.79              |
| 13:V:262:GLU:HG3  | 14:W:202:LYS:NZ   | 1.97                     | 0.79              |
| 13:V:239:GLU:HA   | 13:V:243:GLU:CB   | 2.12                     | 0.79              |
| 1:E:81:ARG:HG2    | 3:G:58:THR:CG2    | 2.13                     | 0.79              |
| 13:V:261:ARG:O    | 14:W:198:LYS:HE3  | 1.83                     | 0.79              |
| 5:I:126:LYS:HE3   | 13:V:216:PRO:HB2  | 1.63                     | 0.79              |
| 9:M:235:ILE:HG22  | 9:M:235:ILE:O     | 1.83                     | 0.79              |
| 1:E:81:ARG:HG2    | 3:G:58:THR:HG21   | 1.63                     | 0.78              |
| 4:H:46:ILE:HG22   | 4:H:50:ILE:HG21   | 1.65                     | 0.78              |
| 5:I:116:GLU:O     | 13:V:232:ARG:NH2  | 2.16                     | 0.78              |
| 7:K:224:LYS:HB3   | 8:L:122:PHE:CE2   | 2.17                     | 0.78              |
| 1:A:56:LEU:O      | 1:A:60:THR:HG23   | 1.84                     | 0.78              |
| 1:A:56:LEU:HD21   | 2:B:67:PHE:N      | 1.97                     | 0.78              |
| 3:G:73:GLU:HA     | 4:H:23:ARG:NH2    | 1.99                     | 0.78              |
| 13:V:133:VAL:HG21 | 13:V:168:ASP:HA   | 1.63                     | 0.78              |
| 7:K:110:ASN:OD1   | 7:K:124:ARG:NH1   | 2.17                     | 0.78              |
| 7:K:378:THR:HG22  | 7:K:379:ARG:H     | 1.48                     | 0.78              |
| 1:E:64:GLU:HB2    | 2:F:45:VAL:CG1    | 2.13                     | 0.78              |
| 1:A:13:ALA:HB3    | 5:I:164:LYS:HD2   | 1.64                     | 0.77              |
| 7:K:193:LEU:HB2   | 7:K:268:LEU:HD22  | 1.65                     | 0.77              |
| 10:N:37:LEU:O     | 10:N:54:ARG:HG3   | 1.83                     | 0.77              |
| 15:X:136:DG:H5''  | 15:X:136:DG:C8    | 2.19                     | 0.77              |
| 5:I:118:PHE:CD2   | 13:V:247:LEU:HD13 | 2.19                     | 0.77              |
| 15:X:57:DT:H6     | 15:X:57:DT:H5'    | 1.50                     | 0.77              |
| 15:X:126:DC:H1'   | 15:X:127:DT:H5'   | 1.67                     | 0.77              |
| 5:I:1983:VAL:HG23 | 9:O:238:VAL:CG1   | 2.14                     | 0.77              |
| 1:A:55:VAL:HG13   | 2:B:107:ALA:HB1   | 1.67                     | 0.77              |
| 1:A:84:LEU:HD13   | 2:B:58:ILE:HG21   | 1.64                     | 0.77              |
| 13:V:190:ASP:OD1  | 13:V:190:ASP:N    | 2.14                     | 0.77              |
| 15:X:75:DG:H1     | 16:Y:-75:DC:H42   | 1.29                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:X:141:DC:H2''  | 15:X:142:DT:H5'   | 1.67                     | 0.77              |
| 1:A:13:ALA:CB     | 5:I:164:LYS:HD3   | 1.96                     | 0.77              |
| 2:B:34:TYR:H      | 2:B:60:ASN:HD21   | 1.33                     | 0.77              |
| 7:K:220:MET:HE2   | 8:L:123:PRO:HD3   | 1.67                     | 0.77              |
| 7:K:92:ASN:HB3    | 7:K:120:GLN:HB3   | 1.67                     | 0.77              |
| 1:A:55:VAL:O      | 1:A:59:LEU:HG     | 1.85                     | 0.77              |
| 7:K:238:LEU:HG    | 7:K:266:GLN:HB2   | 1.67                     | 0.77              |
| 7:K:277:VAL:HB    | 7:K:278:PRO:HD3   | 1.65                     | 0.77              |
| 7:K:332:ARG:O     | 7:K:336:GLU:HG2   | 1.84                     | 0.77              |
| 1:A:31:VAL:HG13   | 2:B:67:PHE:CE2    | 2.20                     | 0.77              |
| 5:I:923:PHE:CE1   | 10:N:201:LYS:NZ   | 2.52                     | 0.77              |
| 16:Y:-53:DG:H4'   | 16:Y:-52:DC:OP1   | 1.82                     | 0.77              |
| 3:C:127:ALA:O     | 3:C:131:ARG:HG3   | 1.84                     | 0.76              |
| 9:M:113:MET:HG3   | 9:M:276:ARG:HH11  | 1.49                     | 0.76              |
| 5:I:2037:LEU:HD11 | 5:I:2039:GLN:HG2  | 1.66                     | 0.76              |
| 13:V:237:THR:CG2  | 13:V:238:PRO:HD3  | 2.13                     | 0.76              |
| 15:X:7:DG:H1'     | 15:X:8:DT:H5''    | 1.67                     | 0.76              |
| 5:I:915:PRO:O     | 9:O:128:LYS:NZ    | 2.18                     | 0.76              |
| 15:X:136:DG:H2''  | 15:X:137:DG:O4'   | 1.85                     | 0.76              |
| 1:E:20:ARG:CD     | 2:F:121:SER:OG    | 2.32                     | 0.76              |
| 13:V:208:VAL:HG13 | 13:V:209:PRO:HD3  | 1.68                     | 0.76              |
| 5:I:163:ARG:C     | 5:I:166:VAL:HG22  | 2.11                     | 0.76              |
| 7:K:155:THR:HG23  | 7:K:173:ILE:HB    | 1.68                     | 0.76              |
| 5:I:120:SER:HB2   | 13:V:233:LEU:HD12 | 1.66                     | 0.76              |
| 1:A:33:ARG:HA     | 1:A:36:ARG:CG     | 2.15                     | 0.76              |
| 7:K:121:ALA:HB2   | 7:K:376:VAL:HG22  | 1.66                     | 0.76              |
| 7:K:224:LYS:HB3   | 8:L:122:PHE:CZ    | 2.21                     | 0.76              |
| 10:N:123:PHE:CE1  | 10:N:324:LEU:HD23 | 2.21                     | 0.76              |
| 15:X:139:DT:H2''  | 15:X:140:DT:H5'   | 1.66                     | 0.76              |
| 13:V:239:GLU:CD   | 13:V:240:GLN:HG2  | 2.10                     | 0.75              |
| 15:X:53:DC:H2''   | 15:X:54:DG:C8     | 2.19                     | 0.75              |
| 7:K:70:VAL:O      | 7:K:74:VAL:HG23   | 1.86                     | 0.75              |
| 1:A:35:LEU:HD21   | 2:B:67:PHE:CE1    | 2.21                     | 0.75              |
| 1:A:58:TYR:OH     | 2:B:106:HIS:ND1   | 2.18                     | 0.75              |
| 1:E:57:TYR:HA     | 6:J:130:ARG:NH1   | 2.00                     | 0.75              |
| 15:X:59:DA:H2''   | 15:X:60:DA:H5''   | 1.65                     | 0.75              |
| 5:I:660:LEU:HD23  | 5:I:742:TYR:CE2   | 2.22                     | 0.75              |
| 5:I:930:LEU:HD21  | 10:N:250:ILE:HD12 | 1.66                     | 0.75              |
| 15:X:99:DA:H1'    | 15:X:100:DG:H5'   | 1.67                     | 0.75              |
| 7:K:175:VAL:HA    | 7:K:179:LEU:HD22  | 1.69                     | 0.75              |
| 13:V:94:PRO:O     | 13:V:117:ALA:HB2  | 1.86                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:51:TYR:HB3    | 2:B:91:ILE:HG21   | 1.69                     | 0.75              |
| 7:K:375:MET:O     | 7:K:376:VAL:HG12  | 1.86                     | 0.75              |
| 1:A:55:VAL:HG12   | 1:A:59:LEU:HD21   | 1.67                     | 0.75              |
| 7:K:212:VAL:HG12  | 7:K:332:ARG:HG3   | 1.69                     | 0.75              |
| 13:V:119:GLU:OE1  | 13:V:119:GLU:N    | 2.19                     | 0.75              |
| 5:I:2014:LEU:HD11 | 9:Q:256:ILE:HG13  | 1.68                     | 0.74              |
| 5:I:2088:ARG:HG3  | 5:I:2115:ILE:O    | 1.87                     | 0.74              |
| 10:N:231:GLU:HB2  | 10:N:234:LYS:HE3  | 1.67                     | 0.74              |
| 13:V:169:LEU:HD21 | 13:V:195:TYR:CZ   | 2.22                     | 0.74              |
| 16:Y:-14:DA:H2''  | 16:Y:-13:DT:C5    | 2.22                     | 0.74              |
| 13:V:156:GLU:OE1  | 13:V:183:PHE:CD1  | 2.40                     | 0.74              |
| 10:R:205:LEU:HG   | 10:R:225:VAL:HG22 | 1.70                     | 0.74              |
| 3:C:51:ILE:HD11   | 4:D:44:LYS:HA     | 1.70                     | 0.74              |
| 5:I:754:PHE:CD1   | 5:I:755:LYS:HG3   | 2.22                     | 0.74              |
| 7:K:216:PHE:O     | 7:K:220:MET:HG2   | 1.87                     | 0.74              |
| 5:I:842:LYS:HE3   | 5:I:849:MET:HE3   | 1.69                     | 0.74              |
| 7:K:99:TYR:OH     | 7:K:158:VAL:HG21  | 1.88                     | 0.74              |
| 9:M:172:LEU:HD21  | 9:M:193:ILE:HD13  | 1.70                     | 0.74              |
| 15:X:3:DG:C2'     | 15:X:4:DG:H5'     | 2.18                     | 0.74              |
| 16:Y:-26:DG:H2''  | 16:Y:-25:DG:C8    | 2.23                     | 0.74              |
| 7:K:144:CYS:HA    | 7:K:160:TYR:O     | 1.87                     | 0.74              |
| 1:E:68:ASN:ND2    | 1:E:71:ARG:HB3    | 2.03                     | 0.74              |
| 2:B:87:THR:OG1    | 2:B:90:GLU:OE1    | 2.05                     | 0.73              |
| 7:K:304:ASN:ND2   | 7:K:306:PRO:HD2   | 2.03                     | 0.73              |
| 9:M:313:THR:HG21  | 10:R:303:MET:HG3  | 1.68                     | 0.73              |
| 3:G:107:THR:CG2   | 3:G:124:ILE:HG12  | 2.18                     | 0.73              |
| 5:I:95:GLU:OE2    | 13:V:261:ARG:NH2  | 2.20                     | 0.73              |
| 5:I:1886:LEU:HD21 | 7:K:315:LYS:HE2   | 1.69                     | 0.73              |
| 1:A:27:PRO:HD2    | 2:B:34:TYR:HE1    | 1.52                     | 0.73              |
| 15:X:54:DG:H2'    | 15:X:54:DG:OP2    | 1.89                     | 0.73              |
| 1:E:39:TYR:O      | 2:F:75:SER:HB2    | 1.88                     | 0.73              |
| 16:Y:-23:DA:H2'   | 16:Y:-22:DC:C6    | 2.23                     | 0.73              |
| 4:H:39:ARG:NH1    | 4:H:46:ILE:HD11   | 2.04                     | 0.73              |
| 5:I:116:GLU:CD    | 13:V:240:GLN:HG3  | 2.13                     | 0.73              |
| 7:K:298:ILE:O     | 7:K:302:ILE:HG12  | 1.88                     | 0.73              |
| 10:R:114:SER:OG   | 10:R:117:GLU:OE1  | 2.06                     | 0.73              |
| 13:V:222:HIS:HA   | 13:V:225:ARG:HD3  | 1.71                     | 0.73              |
| 7:K:88:PHE:HB3    | 7:K:119:PHE:HD2   | 1.54                     | 0.73              |
| 7:K:123:LEU:HA    | 7:K:394:PHE:CZ    | 2.24                     | 0.73              |
| 7:K:237:VAL:HG11  | 7:K:250:LYS:HE2   | 1.71                     | 0.73              |
| 5:I:621:TYR:HE2   | 5:I:846:GLU:CD    | 1.97                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:K:302:ILE:HG22  | 7:K:310:GLN:HB3   | 1.69                     | 0.73              |
| 15:X:55:DG:H2''   | 15:X:56:DT:H5''   | 1.70                     | 0.73              |
| 15:X:97:DC:H6     | 15:X:97:DC:H5''   | 1.54                     | 0.73              |
| 3:C:130:ILE:HD13  | 3:G:127:ALA:HA    | 1.71                     | 0.72              |
| 1:E:20:ARG:HG2    | 2:F:121:SER:OG    | 1.87                     | 0.72              |
| 5:I:128:PRO:HB3   | 13:V:216:PRO:HG2  | 1.71                     | 0.72              |
| 7:K:302:ILE:HG21  | 7:K:314:PHE:CD1   | 2.23                     | 0.72              |
| 7:K:377:VAL:CG2   | 7:K:393:LYS:HG3   | 2.19                     | 0.72              |
| 15:X:10:DT:H1'    | 15:X:11:DA:H5'    | 1.72                     | 0.72              |
| 1:A:32:HIS:ND1    | 1:A:49:PRO:HG3    | 2.05                     | 0.72              |
| 7:K:56:TYR:HB2    | 8:L:39:ASN:CG     | 2.14                     | 0.72              |
| 15:X:114:DC:H1'   | 15:X:115:DA:C8    | 2.25                     | 0.72              |
| 1:A:81:PRO:HB2    | 1:A:105:GLN:O     | 1.89                     | 0.72              |
| 3:G:103:LEU:HD21  | 3:G:128:ARG:HD2   | 1.71                     | 0.72              |
| 9:M:35:ALA:CB     | 9:M:40:VAL:HG22   | 2.20                     | 0.72              |
| 13:V:96:LYS:CD    | 13:V:98:MET:HG2   | 2.18                     | 0.72              |
| 13:V:169:LEU:HD11 | 13:V:195:TYR:OH   | 1.89                     | 0.72              |
| 4:D:92:ARG:HH21   | 2:F:98:LEU:HD23   | 1.55                     | 0.72              |
| 5:I:116:GLU:OE1   | 13:V:240:GLN:HG3  | 1.89                     | 0.72              |
| 5:I:2063:LEU:HD11 | 5:I:2127:LEU:HD23 | 1.70                     | 0.72              |
| 13:V:139:SER:HB3  | 13:V:142:GLU:HG3  | 1.72                     | 0.72              |
| 15:X:87:DT:H1'    | 15:X:88:DT:C6     | 2.25                     | 0.72              |
| 1:E:65:LEU:HB3    | 1:E:86:ALA:HB1    | 1.72                     | 0.72              |
| 10:N:301:VAL:HG21 | 10:N:326:MET:CB   | 2.18                     | 0.72              |
| 7:K:36:ARG:NE     | 7:K:36:ARG:HA     | 2.04                     | 0.72              |
| 1:A:41:ALA:HB2    | 2:B:86:ILE:HG13   | 1.70                     | 0.71              |
| 2:F:99:LEU:HB2    | 2:F:104:ALA:HB2   | 1.70                     | 0.71              |
| 5:I:2037:LEU:HD13 | 5:I:2081:TYR:CE2  | 2.24                     | 0.71              |
| 10:N:38:GLU:CD    | 10:N:54:ARG:NH1   | 2.48                     | 0.71              |
| 5:I:667:TRP:CE2   | 5:I:719:HIS:CE1   | 2.78                     | 0.71              |
| 13:V:262:GLU:HG3  | 14:W:202:LYS:HZ2  | 1.54                     | 0.71              |
| 16:Y:-22:DC:H2''  | 16:Y:-21:DG:H8    | 1.54                     | 0.71              |
| 1:A:32:HIS:HB2    | 1:A:49:PRO:CB     | 2.20                     | 0.71              |
| 1:A:116:LEU:CD1   | 3:C:108:ASN:HD21  | 2.03                     | 0.71              |
| 16:Y:-52:DC:H2''  | 16:Y:-51:DC:O5'   | 1.89                     | 0.71              |
| 7:K:302:ILE:HG21  | 7:K:314:PHE:CE1   | 2.26                     | 0.71              |
| 5:I:901:CYS:O     | 5:I:2044:LYS:HE3  | 1.90                     | 0.71              |
| 16:Y:-101:DT:H2'' | 16:Y:-100:DC:H5'  | 1.72                     | 0.71              |
| 16:Y:-10:DA:H2''  | 16:Y:-9:DT:H5''   | 1.71                     | 0.71              |
| 2:B:117:LYS:HE2   | 2:B:122:LYS:HD2   | 1.72                     | 0.71              |
| 1:A:27:PRO:HD2    | 2:B:34:TYR:CE1    | 2.26                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:K:82:GLU:HG2    | 7:K:83:MET:HG2    | 1.71                     | 0.71              |
| 7:K:133:HIS:CE1   | 7:K:137:ARG:HD2   | 2.26                     | 0.71              |
| 15:X:36:DG:H2''   | 15:X:37:DG:OP2    | 1.90                     | 0.71              |
| 3:G:107:THR:HG21  | 3:G:124:ILE:HG12  | 1.73                     | 0.70              |
| 13:V:261:ARG:HB3  | 13:V:262:GLU:OE2  | 1.91                     | 0.70              |
| 7:K:93:ILE:O      | 7:K:122:VAL:HA    | 1.91                     | 0.70              |
| 13:V:124:TYR:CD1  | 13:V:125:PRO:HD2  | 2.25                     | 0.70              |
| 5:I:969:LEU:HB2   | 10:R:225:VAL:HA   | 1.72                     | 0.70              |
| 7:K:314:PHE:HZ    | 7:K:345:TYR:HD2   | 1.39                     | 0.70              |
| 13:V:258:LYS:HB3  | 13:V:259:LYS:HZ2  | 1.54                     | 0.70              |
| 5:I:2014:LEU:HD11 | 9:Q:259:MET:SD    | 2.31                     | 0.70              |
| 5:I:916:PHE:HB3   | 5:I:1983:VAL:HG22 | 1.71                     | 0.70              |
| 13:V:147:LEU:CD1  | 13:V:198:ILE:HG23 | 2.21                     | 0.70              |
| 16:Y:-98:DA:H2''  | 16:Y:-97:DG:H8    | 1.57                     | 0.70              |
| 1:A:41:ALA:HB2    | 2:B:86:ILE:CG1    | 2.21                     | 0.70              |
| 16:Y:-142:DA:H1'  | 16:Y:-141:DG:H5'  | 1.72                     | 0.70              |
| 7:K:377:VAL:HG23  | 7:K:393:LYS:HG3   | 1.74                     | 0.70              |
| 7:K:309:MET:HG2   | 7:K:313:PHE:CE2   | 2.26                     | 0.70              |
| 13:V:96:LYS:O     | 13:V:98:MET:HG3   | 1.91                     | 0.70              |
| 16:Y:-44:DA:H2'   | 16:Y:-43:DT:H72   | 1.72                     | 0.70              |
| 3:G:74:ILE:HD13   | 4:H:62:LEU:HB3    | 1.74                     | 0.70              |
| 7:K:218:ARG:O     | 7:K:222:ILE:HG12  | 1.91                     | 0.70              |
| 9:M:110:GLU:CG    | 9:M:269:THR:HG22  | 2.19                     | 0.70              |
| 16:Y:-54:DC:H2''  | 16:Y:-53:DG:C8    | 2.27                     | 0.70              |
| 7:K:114:PHE:HE1   | 7:K:122:VAL:HB    | 1.56                     | 0.69              |
| 7:K:152:TYR:CZ    | 7:K:178:LYS:HG2   | 2.27                     | 0.69              |
| 15:X:59:DA:H2''   | 15:X:60:DA:C5'    | 2.22                     | 0.69              |
| 3:G:74:ILE:HG23   | 4:H:63:GLU:HG2    | 1.74                     | 0.69              |
| 7:K:150:SER:HB2   | 7:K:323:ASN:HB2   | 1.74                     | 0.69              |
| 3:C:61:LEU:HD12   | 4:D:37:LEU:HD23   | 1.74                     | 0.69              |
| 5:I:1992:ALA:HB2  | 10:N:201:LYS:NZ   | 2.06                     | 0.69              |
| 7:K:120:GLN:N     | 7:K:120:GLN:HE21  | 1.90                     | 0.69              |
| 1:A:26:PHE:CZ     | 1:A:60:THR:HG21   | 2.27                     | 0.69              |
| 5:I:694:LYS:HB2   | 5:I:719:HIS:HD2   | 1.56                     | 0.69              |
| 1:A:41:ALA:HB2    | 2:B:86:ILE:CD1    | 2.22                     | 0.69              |
| 5:I:1983:VAL:CG2  | 9:O:238:VAL:CG1   | 2.61                     | 0.69              |
| 13:V:239:GLU:O    | 13:V:243:GLU:N    | 2.25                     | 0.69              |
| 3:G:118:THR:OG1   | 4:H:45:ARG:HD3    | 1.90                     | 0.69              |
| 5:I:141:CYS:O     | 5:I:145:GLN:HG3   | 1.92                     | 0.69              |
| 16:Y:-98:DA:H2''  | 16:Y:-97:DG:C8    | 2.27                     | 0.69              |
| 1:E:92:GLU:HG2    | 2:F:103:LEU:HB2   | 1.75                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:G:116:ARG:NH2   | 3:G:123:ASP:OD1   | 2.25                     | 0.69              |
| 5:I:2154:ARG:NH1  | 17:I:3301:ADP:O2A | 2.26                     | 0.69              |
| 7:K:156:HIS:CD2   | 7:K:170:ILE:HD11  | 2.28                     | 0.69              |
| 13:V:261:ARG:HD2  | 14:W:198:LYS:HG2  | 1.73                     | 0.69              |
| 16:Y:-146:DC:H5'  | 16:Y:-146:DC:C6   | 2.27                     | 0.69              |
| 16:Y:-10:DA:H2''  | 16:Y:-9:DT:C5'    | 2.23                     | 0.69              |
| 1:E:21:ALA:C      | 2:F:117:LYS:HD3   | 2.18                     | 0.69              |
| 7:K:335:SER:HA    | 7:K:338:ARG:HE    | 1.58                     | 0.69              |
| 5:I:2060:HIS:CD2  | 5:I:2131:ASP:OD2  | 2.46                     | 0.69              |
| 5:I:2088:ARG:HD3  | 5:I:2115:ILE:CG2  | 2.23                     | 0.69              |
| 7:K:108:SER:O     | 7:K:112:ILE:HD12  | 1.93                     | 0.69              |
| 5:I:633:TYR:CD1   | 5:I:742:TYR:CE1   | 2.78                     | 0.68              |
| 5:I:923:PHE:CD1   | 10:N:201:LYS:NZ   | 2.61                     | 0.68              |
| 5:I:2063:LEU:HD21 | 5:I:2127:LEU:HD22 | 1.66                     | 0.68              |
| 7:K:239:PRO:HD3   | 7:K:247:GLY:CA    | 2.22                     | 0.68              |
| 16:Y:-99:DT:H2''  | 16:Y:-98:DA:H5''  | 1.75                     | 0.68              |
| 1:A:88:ILE:HG12   | 1:A:98:LEU:HD12   | 1.74                     | 0.68              |
| 7:K:221:ASP:HA    | 7:K:224:LYS:HZ2   | 1.58                     | 0.68              |
| 10:N:90:MET:HE1   | 10:N:325:ILE:CD1  | 2.24                     | 0.68              |
| 13:V:105:ARG:NH2  | 13:V:107:ASP:OD2  | 2.25                     | 0.68              |
| 1:A:80:ILE:HG13   | 1:A:82:ARG:HB3    | 1.75                     | 0.68              |
| 9:M:413:ALA:CB    | 9:M:433:ILE:HD12  | 2.23                     | 0.68              |
| 2:F:51:ILE:HG21   | 2:F:56:MET:HE2    | 1.75                     | 0.68              |
| 5:I:930:LEU:HD21  | 10:N:250:ILE:CD1  | 2.24                     | 0.68              |
| 13:V:239:GLU:HA   | 13:V:243:GLU:H    | 1.58                     | 0.68              |
| 15:X:141:DC:H2'   | 15:X:142:DT:H71   | 1.73                     | 0.68              |
| 7:K:295:PRO:O     | 7:K:299:VAL:HG23  | 1.93                     | 0.68              |
| 7:K:374:ASP:HB2   | 7:K:375:MET:HE2   | 1.74                     | 0.68              |
| 5:I:2088:ARG:HD3  | 5:I:2115:ILE:HG21 | 1.76                     | 0.68              |
| 7:K:220:MET:O     | 7:K:224:LYS:HG2   | 1.94                     | 0.68              |
| 2:F:53:SER:N      | 16:Y:-127:DA:OP1  | 2.20                     | 0.68              |
| 7:K:282:PHE:O     | 7:K:284:PRO:HD3   | 1.93                     | 0.68              |
| 9:M:313:THR:CA    | 9:M:316:HIS:HE1   | 1.80                     | 0.68              |
| 13:V:92:VAL:O     | 13:V:94:PRO:HD3   | 1.94                     | 0.68              |
| 5:I:621:TYR:CZ    | 5:I:846:GLU:OE1   | 2.47                     | 0.68              |
| 5:I:917:ILE:HD12  | 9:O:128:LYS:NZ    | 2.09                     | 0.68              |
| 13:V:55:ARG:NH2   | 15:X:39:DA:H5''   | 2.10                     | 0.68              |
| 5:I:118:PHE:CE2   | 13:V:247:LEU:HD13 | 2.30                     | 0.67              |
| 10:R:117:GLU:OE1  | 10:R:117:GLU:N    | 2.27                     | 0.67              |
| 15:X:73:DG:H1'    | 15:X:74:DC:H5'    | 1.74                     | 0.67              |
| 1:A:66:LEU:HD12   | 1:A:94:LEU:HD12   | 1.76                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:I:949:ILE:CD1  | 9:M:249:ARG:O    | 2.41                     | 0.67              |
| 7:K:146:ILE:HB   | 7:K:148:VAL:HG23 | 1.75                     | 0.67              |
| 7:K:312:HIS:HA   | 7:K:315:LYS:HE3  | 1.76                     | 0.67              |
| 13:V:95:TRP:CE2  | 13:V:116:ARG:HG2 | 2.30                     | 0.67              |
| 13:V:179:ASP:O   | 13:V:183:PHE:HB2 | 1.93                     | 0.67              |
| 7:K:233:MET:HG2  | 7:K:252:ARG:CD   | 2.24                     | 0.67              |
| 1:A:30:ARG:HH22  | 2:B:34:TYR:HA    | 1.59                     | 0.67              |
| 4:H:97:LEU:HD11  | 4:H:100:PHE:CD1  | 2.30                     | 0.67              |
| 7:K:319:LEU:HD21 | 7:K:333:VAL:HG11 | 1.75                     | 0.67              |
| 9:M:26:LEU:CD2   | 9:M:30:GLY:O     | 2.31                     | 0.67              |
| 13:V:257:ARG:O   | 13:V:261:ARG:HG2 | 1.94                     | 0.67              |
| 15:X:131:DC:H2'' | 15:X:132:DA:C8   | 2.30                     | 0.67              |
| 7:K:157:ILE:HG21 | 7:K:298:ILE:HA   | 1.76                     | 0.67              |
| 7:K:302:ILE:HD12 | 7:K:313:PHE:HB3  | 1.77                     | 0.67              |
| 5:I:2088:ARG:NH1 | 5:I:2090:ASP:OD1 | 2.28                     | 0.67              |
| 7:K:165:LYS:HZ2  | 7:K:167:LYS:HD3  | 1.59                     | 0.67              |
| 7:K:232:VAL:HG22 | 7:K:233:MET:H    | 1.58                     | 0.67              |
| 15:X:68:DG:H2'   | 15:X:68:DG:OP2   | 1.94                     | 0.67              |
| 16:Y:-3:DC:H2'   | 16:Y:-2:DT:C5    | 2.30                     | 0.67              |
| 1:E:35:ARG:HB3   | 1:E:43:VAL:CG2   | 2.24                     | 0.67              |
| 1:E:49:VAL:HG21  | 2:F:118:TYR:CD2  | 2.30                     | 0.67              |
| 3:G:107:THR:OG1  | 3:G:124:ILE:HG12 | 1.94                     | 0.67              |
| 6:J:260:ARG:HB2  | 10:P:210:THR:HB  | 1.75                     | 0.67              |
| 7:K:120:GLN:CA   | 7:K:378:THR:HG21 | 2.25                     | 0.67              |
| 15:X:123:DG:H2'' | 15:X:124:DG:H8   | 1.60                     | 0.67              |
| 1:E:117:PRO:HD3  | 3:G:48:LEU:CD1   | 2.25                     | 0.67              |
| 7:K:16:GLY:HA2   | 7:K:84:TYR:OH    | 1.94                     | 0.67              |
| 15:X:136:DG:H2'  | 15:X:137:DG:C8   | 2.30                     | 0.66              |
| 1:A:52:LEU:HD21  | 2:B:67:PHE:CE2   | 2.30                     | 0.66              |
| 7:K:361:GLU:O    | 7:K:365:LEU:HD22 | 1.95                     | 0.66              |
| 10:P:68:ILE:HD13 | 10:P:68:ILE:H    | 1.60                     | 0.66              |
| 15:X:81:DG:H2'   | 15:X:82:DT:H71   | 1.78                     | 0.66              |
| 3:G:82:LEU:HD11  | 4:H:70:VAL:HG13  | 1.77                     | 0.66              |
| 7:K:198:GLU:HB2  | 7:K:201:VAL:HG23 | 1.76                     | 0.66              |
| 7:K:265:GLU:HB2  | 7:K:267:ILE:HG23 | 1.77                     | 0.66              |
| 15:X:79:DA:H2''  | 15:X:80:DC:C5    | 2.29                     | 0.66              |
| 5:I:694:LYS:H    | 5:I:719:HIS:CD2  | 2.13                     | 0.66              |
| 7:K:68:TRP:HE1   | 7:K:112:ILE:HD13 | 1.61                     | 0.66              |
| 15:X:44:DT:H2''  | 15:X:45:DC:H5''  | 1.78                     | 0.66              |
| 16:Y:-87:DA:H2'' | 16:Y:-86:DA:C8   | 2.31                     | 0.66              |
| 5:I:936:HIS:CE1  | 10:N:279:LYS:HZ1 | 1.81                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:I:1886:LEU:HD11 | 7:K:311:PRO:HB2    | 1.78                     | 0.66              |
| 5:I:2063:LEU:CD2  | 5:I:2127:LEU:HD23  | 2.16                     | 0.66              |
| 7:K:230:ASN:ND2   | 7:K:232:VAL:HB     | 2.08                     | 0.66              |
| 13:V:265:SER:OG   | 14:W:195:ALA:HA    | 1.95                     | 0.66              |
| 1:A:63:ILE:CG2    | 2:B:59:MET:HE1     | 2.25                     | 0.66              |
| 2:F:33:SER:HB2    | 2:F:60:ASN:OD1     | 1.95                     | 0.66              |
| 7:K:292:MET:HE3   | 7:K:292:MET:O      | 1.96                     | 0.66              |
| 1:A:30:ARG:HG3    | 1:A:33:ARG:HH21    | 1.60                     | 0.66              |
| 3:C:120:MET:HB3   | 3:C:122:LYS:HD2    | 1.77                     | 0.66              |
| 13:V:163:LEU:HD22 | 13:V:167:PHE:HE2   | 1.60                     | 0.66              |
| 13:V:244:GLU:HA   | 13:V:247:LEU:CD2   | 2.26                     | 0.66              |
| 5:I:819:GLN:O     | 5:I:821:TYR:N      | 2.29                     | 0.66              |
| 5:I:1914:LEU:HD13 | 9:M:282:VAL:HG11   | 1.77                     | 0.66              |
| 7:K:74:VAL:O      | 7:K:78:LEU:HG      | 1.96                     | 0.66              |
| 7:K:187:ILE:HA    | 7:K:190:TYR:CD2    | 2.30                     | 0.66              |
| 13:V:265:SER:CB   | 14:W:198:LYS:HD3   | 2.26                     | 0.66              |
| 5:I:622:GLN:CD    | 17:I:3301:ADP:HN61 | 2.04                     | 0.66              |
| 16:Y:-5:DT:C2'    | 16:Y:-4:DC:H5'     | 2.23                     | 0.66              |
| 3:G:110:CYS:HB2   | 3:G:123:ASP:HB3    | 1.78                     | 0.65              |
| 13:V:239:GLU:O    | 13:V:244:GLU:N     | 2.26                     | 0.65              |
| 5:I:810:PRO:O     | 5:I:814:MET:CG     | 2.37                     | 0.65              |
| 7:K:133:HIS:CG    | 7:K:366:ILE:HG12   | 2.31                     | 0.65              |
| 13:V:268:LEU:HD22 | 14:W:191:SER:CB    | 2.26                     | 0.65              |
| 15:X:100:DG:H1'   | 15:X:101:DA:C8     | 2.31                     | 0.65              |
| 16:Y:-146:DC:H2'  | 16:Y:-145:DT:H72   | 1.79                     | 0.65              |
| 16:Y:-134:DG:H1'  | 16:Y:-133:DG:H5'   | 1.78                     | 0.65              |
| 1:E:20:ARG:HD3    | 2:F:121:SER:OG     | 1.95                     | 0.65              |
| 1:E:85:LEU:O      | 1:E:89:ASN:ND2     | 2.21                     | 0.65              |
| 5:I:921:ILE:HG23  | 5:I:1986:PRO:HD2   | 1.74                     | 0.65              |
| 7:K:287:ILE:HG23  | 8:L:35:LEU:HD13    | 1.79                     | 0.65              |
| 7:K:336:GLU:O     | 7:K:340:LEU:HD22   | 1.95                     | 0.65              |
| 16:Y:-145:DT:H2'' | 16:Y:-144:DG:C5'   | 2.22                     | 0.65              |
| 16:Y:-142:DA:H5'  | 16:Y:-142:DA:H8    | 1.61                     | 0.65              |
| 5:I:1914:LEU:HD13 | 9:M:282:VAL:CG1    | 2.26                     | 0.65              |
| 7:K:38:LYS:HB3    | 7:K:40:PHE:CE1     | 2.32                     | 0.65              |
| 7:K:81:LYS:HA     | 7:K:85:GLN:CA      | 2.20                     | 0.65              |
| 16:Y:-23:DA:H2''  | 16:Y:-22:DC:H5'    | 1.79                     | 0.65              |
| 16:Y:-21:DG:H2'   | 16:Y:-20:DT:C6     | 2.32                     | 0.65              |
| 2:B:89:ARG:CZ     | 13:V:63:SER:HB3    | 2.27                     | 0.65              |
| 3:G:63:ARG:HH21   | 15:X:59:DA:H4'     | 1.62                     | 0.65              |
| 5:I:949:ILE:CG2   | 10:R:260:LEU:HD22  | 2.21                     | 0.65              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:90:GLU:HA     | 2:B:93:THR:HG22  | 1.79                     | 0.65              |
| 4:D:45:ARG:CZ     | 15:X:80:DC:H4'   | 2.26                     | 0.65              |
| 5:I:2014:LEU:CG   | 5:I:2017:ARG:HD2 | 2.27                     | 0.65              |
| 7:K:106:GLN:HA    | 7:K:109:MET:HB3  | 1.77                     | 0.65              |
| 15:X:71:DC:H2''   | 15:X:72:DA:C8    | 2.31                     | 0.65              |
| 15:X:108:DT:H2''  | 15:X:109:DA:C8   | 2.31                     | 0.65              |
| 3:C:128:ARG:NH1   | 3:C:133:GLU:OE1  | 2.23                     | 0.65              |
| 7:K:156:HIS:HD2   | 7:K:170:ILE:HD11 | 1.62                     | 0.65              |
| 7:K:185:LYS:HG2   | 7:K:202:ILE:HG21 | 1.77                     | 0.65              |
| 7:K:220:MET:SD    | 7:K:275:PHE:HE1  | 2.19                     | 0.65              |
| 13:V:247:LEU:HD12 | 13:V:248:LEU:N   | 2.12                     | 0.65              |
| 1:E:114:VAL:HG12  | 3:G:117:VAL:CG2  | 2.27                     | 0.65              |
| 14:W:29:ASN:OD1   | 14:W:116:HIS:NE2 | 2.29                     | 0.65              |
| 7:K:211:TYR:O     | 7:K:275:PHE:HA   | 1.97                     | 0.65              |
| 1:A:21:ARG:HH11   | 1:A:21:ARG:CB    | 2.06                     | 0.64              |
| 1:A:31:VAL:HG13   | 2:B:67:PHE:HE2   | 1.58                     | 0.64              |
| 7:K:107:GLU:HA    | 7:K:110:ASN:ND2  | 2.13                     | 0.64              |
| 7:K:299:VAL:O     | 7:K:303:GLN:HG2  | 1.97                     | 0.64              |
| 5:I:949:ILE:HG21  | 9:M:247:ASN:C    | 2.12                     | 0.64              |
| 7:K:187:ILE:HA    | 7:K:190:TYR:CE2  | 2.32                     | 0.64              |
| 13:V:115:ARG:HB3  | 13:V:119:GLU:OE2 | 1.97                     | 0.64              |
| 16:Y:-112:DT:H1'  | 16:Y:-111:DC:H5' | 1.79                     | 0.64              |
| 16:Y:-39:DT:H2''  | 16:Y:-38:DC:H5'' | 1.78                     | 0.64              |
| 1:A:33:ARG:HA     | 1:A:36:ARG:HG3   | 1.78                     | 0.64              |
| 1:E:42:ARG:HG2    | 15:X:111:DG:H4'  | 1.79                     | 0.64              |
| 1:E:101:THR:HG23  | 4:H:96:THR:O     | 1.97                     | 0.64              |
| 7:K:88:PHE:HB3    | 7:K:119:PHE:CD2  | 2.31                     | 0.64              |
| 5:I:118:PHE:CZ    | 13:V:247:LEU:HB2 | 2.33                     | 0.64              |
| 5:I:657:LEU:HD23  | 5:I:670:HIS:ND1  | 2.11                     | 0.64              |
| 7:K:211:TYR:CE1   | 7:K:274:ARG:HD3  | 2.25                     | 0.64              |
| 15:X:25:DC:OP2    | 15:X:25:DC:H2'   | 1.97                     | 0.64              |
| 15:X:113:DC:H2''  | 15:X:114:DC:O5'  | 1.96                     | 0.64              |
| 1:E:76:THR:O      | 1:E:76:THR:OG1   | 2.16                     | 0.64              |
| 9:M:413:ALA:N     | 9:M:433:ILE:HD13 | 2.13                     | 0.64              |
| 15:X:131:DC:H2''  | 15:X:132:DA:H8   | 1.63                     | 0.64              |
| 5:I:2088:ARG:CD   | 5:I:2115:ILE:CG2 | 2.76                     | 0.64              |
| 7:K:68:TRP:NE1    | 7:K:112:ILE:HD13 | 2.12                     | 0.64              |
| 9:M:96:MET:SD     | 9:M:115:ASN:ND2  | 2.71                     | 0.64              |
| 1:E:81:ARG:O      | 1:E:81:ARG:HD3   | 1.98                     | 0.64              |
| 2:B:88:SER:OG     | 13:V:60:LEU:HD21 | 1.98                     | 0.64              |
| 2:F:77:LEU:HD11   | 2:F:93:THR:CG2   | 2.28                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:K:121:ALA:CB    | 7:K:376:VAL:HG22  | 2.28                     | 0.64              |
| 7:K:233:MET:HA    | 7:K:255:MET:CE    | 2.25                     | 0.64              |
| 7:K:331:ASP:O     | 7:K:335:SER:OG    | 2.16                     | 0.64              |
| 13:V:244:GLU:O    | 13:V:248:LEU:HG   | 1.98                     | 0.64              |
| 13:V:258:LYS:HE3  | 13:V:259:LYS:HG3  | 1.79                     | 0.64              |
| 16:Y:-120:DT:H1'  | 16:Y:-119:DC:H5'  | 1.78                     | 0.64              |
| 7:K:314:PHE:CE2   | 7:K:345:TYR:HB3   | 2.33                     | 0.64              |
| 9:M:56:ILE:HG12   | 9:M:326:ILE:HG21  | 1.80                     | 0.64              |
| 10:N:324:LEU:HD11 | 10:N:326:MET:HE3  | 1.79                     | 0.64              |
| 16:Y:-10:DA:C2'   | 16:Y:-9:DT:H5''   | 2.28                     | 0.64              |
| 1:A:33:ARG:HA     | 1:A:36:ARG:NE     | 2.13                     | 0.63              |
| 1:A:91:ASP:OD1    | 8:L:17:ARG:NH2    | 2.31                     | 0.63              |
| 2:B:75:SER:HB2    | 2:B:86:ILE:HD11   | 1.80                     | 0.63              |
| 3:C:61:LEU:HD11   | 4:D:40:ARG:CZ     | 2.29                     | 0.63              |
| 3:G:102:GLY:O     | 3:G:131:ARG:NH2   | 2.31                     | 0.63              |
| 9:M:235:ILE:O     | 9:M:235:ILE:CG2   | 2.46                     | 0.63              |
| 9:O:447:LEU:HD12  | 10:P:343:PRO:HB3  | 1.79                     | 0.63              |
| 15:X:92:DC:H2''   | 15:X:93:DG:O5'    | 1.97                     | 0.63              |
| 16:Y:-84:DG:H1'   | 16:Y:-83:DC:H5'   | 1.79                     | 0.63              |
| 1:E:56:GLU:HG2    | 6:J:130:ARG:NH2   | 2.13                     | 0.63              |
| 7:K:93:ILE:HD13   | 7:K:113:LEU:HD21  | 1.80                     | 0.63              |
| 7:K:158:VAL:HG22  | 7:K:170:ILE:HD13  | 1.80                     | 0.63              |
| 7:K:376:VAL:HG13  | 7:K:377:VAL:H     | 1.61                     | 0.63              |
| 10:R:247:ILE:HG12 | 10:R:272:VAL:HG22 | 1.80                     | 0.63              |
| 13:V:100:PHE:CD1  | 13:V:113:HIS:HB2  | 2.33                     | 0.63              |
| 13:V:239:GLU:CA   | 13:V:243:GLU:H    | 2.10                     | 0.63              |
| 16:Y:-142:DA:H5'  | 16:Y:-142:DA:C8   | 2.33                     | 0.63              |
| 5:I:2091:GLY:HA3  | 15:X:55:DG:H5'    | 1.80                     | 0.63              |
| 7:K:81:LYS:HB2    | 7:K:85:GLN:NE2    | 2.14                     | 0.63              |
| 9:M:270:GLU:HB2   | 9:M:276:ARG:HE    | 1.62                     | 0.63              |
| 1:A:42:GLU:CG     | 2:B:84:SER:HB2    | 2.28                     | 0.63              |
| 1:A:58:TYR:CE2    | 2:B:106:HIS:HB2   | 2.33                     | 0.63              |
| 3:C:63:ARG:CZ     | 3:C:66:PRO:HG2    | 2.29                     | 0.63              |
| 4:H:39:ARG:HH12   | 4:H:46:ILE:HD11   | 1.62                     | 0.63              |
| 5:I:694:LYS:CB    | 5:I:719:HIS:HD2   | 2.12                     | 0.63              |
| 7:K:222:ILE:O     | 7:K:225:LEU:HB3   | 1.98                     | 0.63              |
| 5:I:732:HIS:HD2   | 5:I:736:ARG:HH12  | 0.65                     | 0.63              |
| 10:R:268:ILE:O    | 10:R:272:VAL:HG23 | 1.99                     | 0.63              |
| 13:V:221:GLY:O    | 13:V:225:ARG:HG3  | 1.98                     | 0.63              |
| 2:F:28:ARG:HG3    | 15:X:123:DG:H5'   | 1.79                     | 0.63              |
| 7:K:334:TYR:HA    | 7:K:349:VAL:HG21  | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:67:GLY:HA2    | 1:E:78:ILE:CG1    | 2.20                     | 0.63              |
| 12:T:338:ILE:CD1  | 13:V:230:LEU:HD22 | 2.29                     | 0.63              |
| 13:V:98:MET:HE1   | 13:V:116:ARG:O    | 1.98                     | 0.63              |
| 5:I:112:GLU:OE1   | 13:V:247:LEU:HD23 | 1.99                     | 0.63              |
| 5:I:613:LEU:CD1   | 6:J:178:ILE:HD13  | 2.29                     | 0.63              |
| 7:K:67:ASN:O      | 7:K:69:ASP:N      | 2.31                     | 0.63              |
| 10:P:305:ASP:OD1  | 10:P:306:ILE:N    | 2.31                     | 0.63              |
| 7:K:4:LEU:HB2     | 7:K:93:ILE:HG13   | 1.81                     | 0.63              |
| 13:V:100:PHE:CE1  | 13:V:113:HIS:HB2  | 2.33                     | 0.63              |
| 1:A:51:TYR:HE1    | 2:B:95:VAL:HG21   | 1.64                     | 0.62              |
| 1:A:56:LEU:HD11   | 2:B:67:PHE:CD2    | 2.34                     | 0.62              |
| 1:A:116:LEU:HD11  | 3:C:108:ASN:ND2   | 2.11                     | 0.62              |
| 5:I:660:LEU:HD21  | 5:I:742:TYR:OH    | 1.96                     | 0.62              |
| 5:I:2037:LEU:HD11 | 5:I:2039:GLN:CG   | 2.29                     | 0.62              |
| 5:I:2063:LEU:CD2  | 5:I:2127:LEU:HD21 | 2.18                     | 0.62              |
| 16:Y:-68:DC:H2''  | 16:Y:-67:DC:C5    | 2.34                     | 0.62              |
| 1:A:89:ARG:HB3    | 1:A:109:LEU:HD11  | 1.80                     | 0.62              |
| 5:I:842:LYS:O     | 5:I:842:LYS:HG2   | 1.99                     | 0.62              |
| 6:J:269:SER:HB3   | 9:Q:150:TYR:CG    | 2.30                     | 0.62              |
| 13:V:91:LYS:NZ    | 13:V:91:LYS:O     | 2.29                     | 0.62              |
| 1:E:73:ASN:O      | 1:E:73:ASN:ND2    | 2.32                     | 0.62              |
| 7:K:335:SER:HA    | 7:K:338:ARG:HH21  | 1.63                     | 0.62              |
| 2:B:90:GLU:HG3    | 4:H:75:HIS:CE1    | 2.34                     | 0.62              |
| 1:E:42:ARG:HB3    | 2:F:85:THR:OG1    | 1.98                     | 0.62              |
| 10:R:305:ASP:OD1  | 10:R:306:ILE:N    | 2.32                     | 0.62              |
| 13:V:167:PHE:O    | 13:V:170:ARG:HG2  | 1.99                     | 0.62              |
| 15:X:11:DA:H2''   | 15:X:12:DT:H5'    | 1.80                     | 0.62              |
| 15:X:94:DG:H2''   | 15:X:95:DT:H5'    | 1.81                     | 0.62              |
| 1:A:33:ARG:CD     | 1:A:37:LYS:HE2    | 2.29                     | 0.62              |
| 5:I:935:VAL:O     | 5:I:936:HIS:ND1   | 2.33                     | 0.62              |
| 7:K:144:CYS:O     | 7:K:316:ASN:HB2   | 1.99                     | 0.62              |
| 10:R:286:GLU:N    | 10:R:286:GLU:OE1  | 2.32                     | 0.62              |
| 13:V:270:LYS:HE2  | 13:V:270:LYS:N    | 2.13                     | 0.62              |
| 2:B:34:TYR:H      | 2:B:60:ASN:ND2    | 1.98                     | 0.62              |
| 5:I:124:LEU:H     | 13:V:226:ARG:HD2  | 1.65                     | 0.62              |
| 5:I:129:GLU:HG3   | 13:V:196:TYR:CE2  | 2.34                     | 0.62              |
| 2:B:75:SER:HA     | 2:B:86:ILE:HD11   | 1.82                     | 0.62              |
| 3:G:90:MET:HE2    | 3:G:90:MET:HA     | 1.82                     | 0.62              |
| 14:W:190:THR:HG22 | 14:W:194:ILE:HD12 | 1.81                     | 0.62              |
| 1:E:117:PRO:HD3   | 3:G:48:LEU:HD11   | 1.82                     | 0.62              |
| 8:L:4:LYS:O       | 8:L:4:LYS:HG2     | 1.99                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:V:268:LEU:HD13 | 14:W:191:SER:HA   | 1.80                     | 0.62              |
| 1:A:56:LEU:HD21   | 2:B:67:PHE:CA     | 2.30                     | 0.62              |
| 1:E:81:ARG:HD3    | 1:E:81:ARG:C      | 2.25                     | 0.62              |
| 3:G:118:THR:HG23  | 4:H:45:ARG:HG2    | 1.82                     | 0.62              |
| 5:I:1914:LEU:HD11 | 9:M:282:VAL:HB    | 1.80                     | 0.62              |
| 7:K:56:TYR:HB3    | 8:L:39:ASN:HD21   | 1.61                     | 0.62              |
| 16:Y:-22:DC:H2''  | 16:Y:-21:DG:C8    | 2.34                     | 0.62              |
| 1:A:26:PHE:CG     | 1:A:57:GLU:HB2    | 2.35                     | 0.62              |
| 1:E:100:VAL:HG11  | 4:H:98:TYR:CE2    | 2.34                     | 0.62              |
| 7:K:228:GLU:O     | 7:K:229:GLU:HG2   | 2.00                     | 0.62              |
| 7:K:364:LYS:O     | 7:K:368:GLU:HG2   | 2.00                     | 0.62              |
| 13:V:90:LYS:O     | 13:V:90:LYS:HG2   | 1.99                     | 0.62              |
| 13:V:220:ALA:HB1  | 13:V:224:ARG:NH2  | 2.15                     | 0.62              |
| 1:A:32:HIS:CG     | 1:A:49:PRO:HG3    | 2.35                     | 0.61              |
| 5:I:106:ILE:HD11  | 13:V:254:ILE:HG22 | 1.80                     | 0.61              |
| 7:K:133:HIS:HE2   | 7:K:365:LEU:HB2   | 1.65                     | 0.61              |
| 9:M:135:VAL:HG22  | 9:M:161:LEU:CD2   | 2.30                     | 0.61              |
| 16:Y:-133:DG:H2'  | 16:Y:-132:DT:H72  | 1.81                     | 0.61              |
| 1:E:18:SER:HB2    | 1:E:25:PHE:O      | 2.00                     | 0.61              |
| 2:F:59:MET:O      | 2:F:63:VAL:HG23   | 2.00                     | 0.61              |
| 13:V:95:TRP:CZ2   | 13:V:116:ARG:HG2  | 2.35                     | 0.61              |
| 13:V:95:TRP:HB3   | 13:V:114:TRP:CZ3  | 2.34                     | 0.61              |
| 1:A:41:ALA:HB2    | 2:B:86:ILE:HD12   | 1.81                     | 0.61              |
| 7:K:165:LYS:HG2   | 7:K:167:LYS:CD    | 2.28                     | 0.61              |
| 7:K:181:THR:O     | 7:K:185:LYS:HG3   | 2.01                     | 0.61              |
| 7:K:185:LYS:HA    | 7:K:202:ILE:HD13  | 1.81                     | 0.61              |
| 13:V:258:LYS:HB3  | 13:V:259:LYS:NZ   | 2.14                     | 0.61              |
| 15:X:123:DG:H2''  | 15:X:124:DG:C8    | 2.35                     | 0.61              |
| 1:A:58:TYR:CZ     | 2:B:106:HIS:HB2   | 2.36                     | 0.61              |
| 2:B:39:TYR:HE1    | 2:B:43:LYS:HE3    | 1.66                     | 0.61              |
| 12:T:190:GLN:OE1  | 12:T:190:GLN:N    | 2.32                     | 0.61              |
| 3:C:42:ARG:HB3    | 3:C:42:ARG:HH11   | 1.65                     | 0.61              |
| 1:E:114:VAL:HG12  | 3:G:117:VAL:HG23  | 1.82                     | 0.61              |
| 15:X:94:DG:H2'    | 15:X:95:DT:C6     | 2.35                     | 0.61              |
| 1:A:29:GLY:O      | 1:A:36:ARG:NH2    | 2.33                     | 0.61              |
| 15:X:43:DA:H2'    | 15:X:44:DT:H72    | 1.82                     | 0.61              |
| 1:A:52:LEU:HD21   | 2:B:67:PHE:CZ     | 2.36                     | 0.61              |
| 2:B:73:GLU:OE2    | 4:H:72:TYR:OH     | 2.13                     | 0.61              |
| 7:K:89:LEU:HD13   | 7:K:89:LEU:H      | 1.65                     | 0.61              |
| 7:K:306:PRO:HB2   | 7:K:309:MET:HB2   | 1.83                     | 0.61              |
| 16:Y:-109:DT:H2'' | 16:Y:-108:DA:N7   | 2.15                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:34:TYR:HB2    | 2:B:60:ASN:ND2    | 2.16                     | 0.61              |
| 2:F:53:SER:H      | 16:Y:-127:DA:P    | 2.22                     | 0.61              |
| 9:Q:254:GLN:OE1   | 9:Q:254:GLN:N     | 2.33                     | 0.61              |
| 13:V:206:ARG:O    | 13:V:208:VAL:N    | 2.33                     | 0.61              |
| 13:V:244:GLU:HB2  | 13:V:247:LEU:HD21 | 1.82                     | 0.61              |
| 13:V:264:ARG:HB3  | 14:W:198:LYS:HE3  | 1.83                     | 0.61              |
| 15:X:8:DT:H2''    | 15:X:9:DA:H5'     | 1.81                     | 0.61              |
| 7:K:26:PRO:HG2    | 7:K:42:ALA:CA     | 2.29                     | 0.60              |
| 7:K:190:TYR:HB2   | 8:L:148:ARG:HH22  | 1.66                     | 0.60              |
| 16:Y:-146:DC:H2'' | 16:Y:-145:DT:C6   | 2.36                     | 0.60              |
| 7:K:225:LEU:HD23  | 7:K:230:ASN:HA    | 1.83                     | 0.60              |
| 9:M:270:GLU:HB2   | 9:M:276:ARG:NE    | 2.15                     | 0.60              |
| 13:V:192:LYS:HB3  | 13:V:218:PHE:CE1  | 2.36                     | 0.60              |
| 16:Y:-102:DC:C2'  | 16:Y:-101:DT:H72  | 2.29                     | 0.60              |
| 6:J:269:SER:HB2   | 9:Q:150:TYR:HB3   | 1.59                     | 0.60              |
| 7:K:149:ASP:O     | 7:K:155:THR:HA    | 2.02                     | 0.60              |
| 7:K:161:CYS:H     | 7:K:166:LYS:HE2   | 1.65                     | 0.60              |
| 10:N:231:GLU:HB2  | 10:N:234:LYS:HE2  | 1.81                     | 0.60              |
| 13:V:96:LYS:HB3   | 13:V:98:MET:CE    | 2.29                     | 0.60              |
| 13:V:235:ASN:O    | 13:V:235:ASN:ND2  | 2.25                     | 0.60              |
| 13:V:259:LYS:HZ2  | 13:V:259:LYS:H    | 1.49                     | 0.60              |
| 15:X:46:DC:H2''   | 15:X:47:DC:C6     | 2.36                     | 0.60              |
| 16:Y:-52:DC:H4'   | 16:Y:-51:DC:OP1   | 2.00                     | 0.60              |
| 5:I:921:ILE:HD13  | 5:I:1986:PRO:CB   | 2.32                     | 0.60              |
| 13:V:147:LEU:HD12 | 13:V:198:ILE:HG23 | 1.82                     | 0.60              |
| 13:V:237:THR:HG23 | 13:V:238:PRO:CD   | 2.25                     | 0.60              |
| 5:I:949:ILE:HG22  | 10:R:260:LEU:CD2  | 2.24                     | 0.60              |
| 13:V:182:GLN:C    | 13:V:183:PHE:CD1  | 2.79                     | 0.60              |
| 16:Y:-44:DA:H2'   | 16:Y:-43:DT:C7    | 2.32                     | 0.60              |
| 16:Y:-3:DC:H2'    | 16:Y:-2:DT:C6     | 2.36                     | 0.60              |
| 2:B:111:GLY:O     | 2:B:115:VAL:HG23  | 2.02                     | 0.60              |
| 1:E:68:ASN:ND2    | 1:E:68:ASN:O      | 2.33                     | 0.60              |
| 1:E:115:LEU:HD22  | 4:H:44:LYS:HG2    | 1.84                     | 0.60              |
| 7:K:123:LEU:HD22  | 7:K:372:PHE:HE1   | 1.65                     | 0.60              |
| 7:K:230:ASN:HD21  | 7:K:232:VAL:HB    | 1.65                     | 0.60              |
| 2:B:41:VAL:O      | 2:B:44:GLN:HG2    | 2.01                     | 0.60              |
| 15:X:13:DA:H2''   | 15:X:14:DT:C5     | 2.36                     | 0.60              |
| 2:B:89:ARG:NE     | 13:V:63:SER:HB3   | 2.17                     | 0.60              |
| 5:I:921:ILE:HG21  | 5:I:1986:PRO:N    | 2.17                     | 0.60              |
| 5:I:694:LYS:H     | 5:I:719:HIS:HD2   | 1.50                     | 0.60              |
| 5:I:754:PHE:HD1   | 5:I:755:LYS:HG3   | 1.65                     | 0.60              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:K:29:GLN:HG3    | 7:K:70:VAL:HG12  | 1.83                     | 0.60              |
| 7:K:232:VAL:HG13  | 7:K:233:MET:N    | 2.16                     | 0.60              |
| 7:K:302:ILE:CD1   | 7:K:313:PHE:HB3  | 2.31                     | 0.60              |
| 1:E:56:GLU:HG3    | 2:F:41:VAL:HG21  | 1.83                     | 0.60              |
| 5:I:613:LEU:HD13  | 6:J:178:ILE:HD13 | 1.84                     | 0.60              |
| 5:I:1954:ALA:HB3  | 9:Q:124:ILE:HD11 | 1.83                     | 0.60              |
| 1:E:20:ARG:HG2    | 1:E:20:ARG:O     | 2.02                     | 0.59              |
| 1:E:102:ILE:HG23  | 2:F:58:ILE:CD1   | 2.31                     | 0.59              |
| 7:K:133:HIS:CD2   | 7:K:366:ILE:HG12 | 2.35                     | 0.59              |
| 7:K:279:GLU:OE2   | 7:K:283:ASN:HB2  | 2.02                     | 0.59              |
| 7:K:319:LEU:HD12  | 7:K:330:ARG:HG2  | 1.82                     | 0.59              |
| 11:U:363:ASP:O    | 13:V:95:TRP:HH2  | 1.85                     | 0.59              |
| 15:X:56:DT:H2''   | 15:X:57:DT:H5''  | 1.84                     | 0.59              |
| 15:X:99:DA:H1'    | 15:X:100:DG:C5'  | 2.31                     | 0.59              |
| 2:B:99:LEU:HB3    | 2:B:103:LEU:HB3  | 1.83                     | 0.59              |
| 5:I:888:MET:SD    | 15:X:51:DG:C6    | 2.95                     | 0.59              |
| 7:K:159:PRO:HA    | 7:K:313:PHE:HE1  | 1.67                     | 0.59              |
| 13:V:257:ARG:HA   | 13:V:260:GLU:HB2 | 1.83                     | 0.59              |
| 7:K:364:LYS:HG2   | 7:K:368:GLU:OE2  | 2.02                     | 0.59              |
| 15:X:51:DG:C1'    | 15:X:52:DG:H5'   | 2.26                     | 0.59              |
| 1:A:33:ARG:HG2    | 1:A:37:LYS:NZ    | 2.17                     | 0.59              |
| 3:G:107:THR:OG1   | 3:G:124:ILE:HA   | 2.02                     | 0.59              |
| 5:I:667:TRP:CD1   | 5:I:719:HIS:ND1  | 2.60                     | 0.59              |
| 7:K:139:ASN:HB3   | 7:K:142:GLU:CG   | 2.32                     | 0.59              |
| 7:K:220:MET:HE3   | 8:L:122:PHE:CD2  | 2.37                     | 0.59              |
| 7:K:356:ILE:HD13  | 7:K:356:ILE:H    | 1.68                     | 0.59              |
| 1:A:52:LEU:HD12   | 1:A:56:LEU:HG    | 1.83                     | 0.59              |
| 3:C:121:PRO:HB3   | 4:D:53:GLU:HG3   | 1.83                     | 0.59              |
| 1:E:35:ARG:HB3    | 1:E:43:VAL:HG21  | 1.85                     | 0.59              |
| 5:I:1972:ILE:HD13 | 10:P:242:VAL:CG1 | 2.32                     | 0.59              |
| 7:K:183:HIS:HD2   | 7:K:277:VAL:HG13 | 1.67                     | 0.59              |
| 7:K:305:LEU:CB    | 7:K:306:PRO:HD3  | 2.32                     | 0.59              |
| 13:V:141:GLN:OE1  | 13:V:141:GLN:N   | 2.35                     | 0.59              |
| 15:X:72:DA:H1'    | 15:X:73:DG:H5'   | 1.84                     | 0.59              |
| 7:K:11:TYR:HB2    | 7:K:152:TYR:CE2  | 2.38                     | 0.59              |
| 7:K:25:ILE:HG22   | 7:K:26:PRO:HD2   | 1.84                     | 0.59              |
| 7:K:314:PHE:HZ    | 7:K:345:TYR:CD2  | 2.21                     | 0.59              |
| 15:X:40:DG:H2''   | 15:X:41:DT:O5'   | 2.03                     | 0.59              |
| 15:X:69:DG:H2''   | 15:X:70:DA:C8    | 2.37                     | 0.59              |
| 7:K:11:TYR:HB2    | 7:K:152:TYR:CD2  | 2.37                     | 0.59              |
| 7:K:101:ASN:ND2   | 7:K:106:GLN:HB2  | 2.17                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:U:364:GLU:O    | 13:V:116:ARG:NH2  | 2.36                     | 0.59              |
| 13:V:246:TYR:HA   | 13:V:249:GLN:NE2  | 2.18                     | 0.59              |
| 3:C:42:ARG:HB3    | 3:C:42:ARG:NH1    | 2.17                     | 0.59              |
| 3:C:115:LYS:HD3   | 3:C:115:LYS:N     | 2.17                     | 0.59              |
| 2:F:28:ARG:HD2    | 2:F:29:SER:H      | 1.68                     | 0.59              |
| 5:I:713:THR:HG1   | 15:X:136:DG:P     | 2.26                     | 0.59              |
| 7:K:15:ILE:HD13   | 7:K:78:LEU:HD13   | 1.85                     | 0.59              |
| 13:V:237:THR:CB   | 13:V:238:PRO:HD3  | 2.33                     | 0.59              |
| 1:A:43:ARG:HG3    | 2:B:85:THR:HB     | 1.85                     | 0.59              |
| 5:I:2088:ARG:CD   | 5:I:2115:ILE:HG22 | 2.33                     | 0.59              |
| 14:W:38:ARG:NH2   | 14:W:41:ASP:OD2   | 2.36                     | 0.59              |
| 15:X:129:DG:H2''  | 15:X:130:DG:C8    | 2.37                     | 0.59              |
| 1:A:84:LEU:HD13   | 2:B:58:ILE:CG2    | 2.32                     | 0.59              |
| 2:B:77:LEU:HD23   | 2:B:93:THR:HG23   | 1.83                     | 0.59              |
| 5:I:1914:LEU:HD22 | 9:M:282:VAL:HG12  | 1.84                     | 0.59              |
| 7:K:159:PRO:CG    | 7:K:169:ALA:HB3   | 2.32                     | 0.59              |
| 7:K:378:THR:HG22  | 7:K:379:ARG:N     | 2.17                     | 0.59              |
| 13:V:264:ARG:CZ   | 14:W:198:LYS:HZ3  | 2.16                     | 0.59              |
| 15:X:141:DC:H6    | 15:X:141:DC:C5'   | 2.16                     | 0.59              |
| 16:Y:-118:DA:H2'' | 16:Y:-117:DA:C8   | 2.36                     | 0.59              |
| 1:A:35:LEU:HD11   | 1:A:52:LEU:CD2    | 2.33                     | 0.58              |
| 1:E:64:GLU:OE1    | 2:F:45:VAL:HG12   | 2.03                     | 0.58              |
| 7:K:212:VAL:CG1   | 7:K:332:ARG:HG3   | 2.32                     | 0.58              |
| 9:M:35:ALA:HB1    | 9:M:40:VAL:HG22   | 1.85                     | 0.58              |
| 15:X:128:DC:H2''  | 15:X:129:DG:C8    | 2.37                     | 0.58              |
| 3:C:49:ARG:HD3    | 15:X:7:DG:P       | 2.44                     | 0.58              |
| 5:I:633:TYR:HD1   | 5:I:742:TYR:CE1   | 2.20                     | 0.58              |
| 5:I:657:LEU:HD22  | 5:I:670:HIS:ND1   | 2.17                     | 0.58              |
| 5:I:935:VAL:O     | 5:I:936:HIS:CG    | 2.56                     | 0.58              |
| 7:K:232:VAL:HG13  | 7:K:233:MET:SD    | 2.43                     | 0.58              |
| 7:K:306:PRO:HB2   | 7:K:309:MET:CB    | 2.33                     | 0.58              |
| 5:I:751:ILE:O     | 5:I:751:ILE:HG22  | 2.03                     | 0.58              |
| 5:I:921:ILE:CD1   | 5:I:1986:PRO:HB2  | 2.33                     | 0.58              |
| 3:G:83:ARG:HE     | 4:H:80:THR:HG22   | 1.69                     | 0.58              |
| 7:K:193:LEU:O     | 7:K:195:VAL:N     | 2.37                     | 0.58              |
| 10:N:165:THR:HG22 | 10:N:228:PRO:HG2  | 1.85                     | 0.58              |
| 10:N:301:VAL:CG2  | 10:N:326:MET:HB2  | 2.33                     | 0.58              |
| 15:X:57:DT:H5'    | 15:X:57:DT:C6     | 2.35                     | 0.58              |
| 16:Y:-104:DA:H2'' | 16:Y:-103:DG:O5'  | 2.02                     | 0.58              |
| 7:K:17:TYR:H      | 7:K:21:ASN:CG     | 2.11                     | 0.58              |
| 7:K:120:GLN:C     | 7:K:378:THR:HG21  | 2.28                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:K:239:PRO:HD3   | 7:K:247:GLY:HA3   | 1.85                     | 0.58              |
| 13:V:113:HIS:HD2  | 13:V:115:ARG:HE   | 1.51                     | 0.58              |
| 3:C:100:LEU:HD11  | 4:D:58:LEU:HD22   | 1.85                     | 0.58              |
| 1:E:111:ILE:HD13  | 3:G:51:ILE:HG21   | 1.85                     | 0.58              |
| 2:F:85:THR:HG22   | 16:Y:-107:DG:OP1  | 2.03                     | 0.58              |
| 13:V:264:ARG:HH22 | 14:W:194:ILE:HG12 | 1.68                     | 0.58              |
| 15:X:87:DT:H1'    | 15:X:88:DT:C5     | 2.38                     | 0.58              |
| 15:X:121:DG:H2''  | 15:X:122:DC:C5    | 2.38                     | 0.58              |
| 15:X:138:DA:H2''  | 15:X:139:DT:H71   | 1.86                     | 0.58              |
| 1:A:51:TYR:CE2    | 2:B:92:GLN:HB2    | 2.39                     | 0.58              |
| 16:Y:-115:DT:H2'' | 16:Y:-114:DG:H8   | 1.67                     | 0.58              |
| 1:A:43:ARG:CG     | 2:B:85:THR:HB     | 2.34                     | 0.58              |
| 5:I:2105:PHE:HE2  | 5:I:2127:LEU:HD21 | 1.68                     | 0.58              |
| 7:K:198:GLU:O     | 7:K:200:HIS:N     | 2.37                     | 0.58              |
| 13:V:147:LEU:HD11 | 13:V:198:ILE:HG23 | 1.85                     | 0.58              |
| 15:X:37:DG:H2''   | 15:X:38:DG:C8     | 2.38                     | 0.58              |
| 16:Y:-146:DC:H2'  | 16:Y:-145:DT:C7   | 2.33                     | 0.58              |
| 16:Y:-86:DA:H2''  | 16:Y:-85:DC:O5'   | 2.02                     | 0.58              |
| 16:Y:-7:DC:H2''   | 16:Y:-6:DA:H5'    | 1.86                     | 0.58              |
| 2:B:89:ARG:NH2    | 13:V:63:SER:HB3   | 2.19                     | 0.58              |
| 5:I:649:LYS:NZ    | 19:I:3303:BEF:F1  | 2.23                     | 0.58              |
| 7:K:205:VAL:HG22  | 7:K:236:TYR:CE1   | 2.39                     | 0.58              |
| 13:V:236:ARG:NH2  | 13:V:240:GLN:O    | 2.32                     | 0.58              |
| 1:A:25:GLN:HG2    | 2:B:40:LYS:HB3    | 1.86                     | 0.58              |
| 2:B:38:VAL:HG11   | 2:B:59:MET:CG     | 2.34                     | 0.58              |
| 3:C:109:LEU:CD1   | 3:G:129:ARG:HG2   | 2.32                     | 0.58              |
| 5:I:163:ARG:O     | 5:I:166:VAL:HG23  | 2.00                     | 0.58              |
| 5:I:726:LYS:HD2   | 15:X:56:DT:H4'    | 1.84                     | 0.58              |
| 7:K:193:LEU:HG    | 7:K:268:LEU:HD13  | 1.86                     | 0.58              |
| 7:K:351:LEU:HD23  | 7:K:352:PRO:O     | 2.03                     | 0.58              |
| 15:X:28:DG:H2''   | 15:X:29:DG:H8     | 1.67                     | 0.58              |
| 15:X:71:DC:H2''   | 15:X:72:DA:H8     | 1.68                     | 0.58              |
| 1:A:25:GLN:OE1    | 2:B:41:VAL:HG22   | 2.03                     | 0.57              |
| 2:B:90:GLU:HA     | 2:B:93:THR:CG2    | 2.34                     | 0.57              |
| 2:F:77:LEU:CD1    | 2:F:93:THR:HB     | 2.34                     | 0.57              |
| 3:G:103:LEU:HD11  | 3:G:128:ARG:CG    | 2.33                     | 0.57              |
| 4:H:49:LEU:H      | 4:H:49:LEU:HD12   | 1.69                     | 0.57              |
| 5:I:2079:LEU:HD12 | 5:I:2115:ILE:HD11 | 1.86                     | 0.57              |
| 7:K:66:VAL:O      | 7:K:67:ASN:ND2    | 2.37                     | 0.57              |
| 7:K:159:PRO:HB3   | 7:K:313:PHE:CZ    | 2.38                     | 0.57              |
| 13:V:50:PRO:C     | 13:V:51:GLU:HG3   | 2.28                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:V:262:GLU:CG   | 14:W:202:LYS:NZ   | 2.65                     | 0.57              |
| 2:B:46:HIS:HB3    | 2:B:49:THR:HB     | 1.86                     | 0.57              |
| 3:C:128:ARG:O     | 3:C:131:ARG:HB2   | 2.04                     | 0.57              |
| 4:H:35:ARG:NH1    | 4:H:35:ARG:HB2    | 2.19                     | 0.57              |
| 9:M:312:PHE:O     | 9:M:316:HIS:ND1   | 2.26                     | 0.57              |
| 15:X:121:DG:H2''  | 15:X:122:DC:C6    | 2.39                     | 0.57              |
| 1:A:35:LEU:HD21   | 2:B:67:PHE:HE1    | 1.63                     | 0.57              |
| 3:G:118:THR:HG23  | 4:H:45:ARG:HB3    | 1.87                     | 0.57              |
| 12:T:12:GLY:H     | 13:V:97:TRP:HH2   | 1.51                     | 0.57              |
| 16:Y:-106:DA:H2'' | 16:Y:-105:DC:C6   | 2.39                     | 0.57              |
| 7:K:32:SER:HB2    | 7:K:54:LEU:CD2    | 2.34                     | 0.57              |
| 7:K:282:PHE:CE2   | 7:K:332:ARG:HB3   | 2.38                     | 0.57              |
| 7:K:376:VAL:O     | 7:K:377:VAL:HB    | 2.04                     | 0.57              |
| 13:V:51:GLU:HB3   | 13:V:58:TYR:CZ    | 2.39                     | 0.57              |
| 13:V:182:GLN:HB2  | 13:V:183:PHE:CE1  | 2.38                     | 0.57              |
| 15:X:118:DT:H2''  | 15:X:119:DG:C8    | 2.39                     | 0.57              |
| 2:B:75:SER:CA     | 2:B:86:ILE:HD11   | 2.34                     | 0.57              |
| 3:G:73:GLU:CA     | 4:H:23:ARG:HH12   | 2.17                     | 0.57              |
| 7:K:1:MET:HE3     | 7:K:92:ASN:CG     | 2.29                     | 0.57              |
| 7:K:159:PRO:HG2   | 7:K:169:ALA:HB3   | 1.85                     | 0.57              |
| 10:P:248:ASP:OD2  | 10:P:273:ARG:NH1  | 2.38                     | 0.57              |
| 10:R:43:SER:O     | 10:R:45:GLY:N     | 2.37                     | 0.57              |
| 7:K:96:THR:HA     | 7:K:125:VAL:O     | 2.05                     | 0.57              |
| 7:K:131:SER:OG    | 7:K:147:ILE:HD12  | 2.04                     | 0.57              |
| 7:K:315:LYS:HA    | 7:K:348:SER:HB3   | 1.86                     | 0.57              |
| 9:M:313:THR:CB    | 9:M:316:HIS:CE1   | 2.88                     | 0.57              |
| 10:N:123:PHE:HE1  | 10:N:324:LEU:HD23 | 1.69                     | 0.57              |
| 13:V:147:LEU:CD1  | 13:V:198:ILE:HA   | 2.35                     | 0.57              |
| 16:Y:-13:DT:H71   | 16:Y:-13:DT:OP2   | 2.04                     | 0.57              |
| 3:G:118:THR:HG23  | 4:H:45:ARG:CG     | 2.35                     | 0.57              |
| 3:G:120:MET:HB2   | 3:G:121:PRO:CD    | 2.35                     | 0.57              |
| 7:K:101:ASN:HD21  | 7:K:106:GLN:H     | 1.51                     | 0.57              |
| 7:K:102:PHE:O     | 7:K:104:SER:N     | 2.37                     | 0.57              |
| 7:K:305:LEU:HB2   | 7:K:306:PRO:HD3   | 1.87                     | 0.57              |
| 13:V:219:ASP:O    | 13:V:223:GLU:HB2  | 2.04                     | 0.57              |
| 13:V:239:GLU:OE2  | 13:V:240:GLN:HG2  | 2.05                     | 0.57              |
| 15:X:48:DC:H1'    | 15:X:49:DT:C6     | 2.40                     | 0.57              |
| 1:A:29:GLY:O      | 1:A:33:ARG:HB2    | 2.05                     | 0.57              |
| 1:E:25:PHE:CD2    | 1:E:26:PRO:HD2    | 2.40                     | 0.57              |
| 7:K:44:GLN:HG3    | 7:K:77:TYR:CE2    | 2.40                     | 0.57              |
| 7:K:68:TRP:O      | 7:K:72:ARG:HG2    | 2.05                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:X:33:DC:H2'    | 15:X:34:DT:H71    | 1.84                     | 0.57              |
| 2:F:77:LEU:HD11   | 2:F:93:THR:HG22   | 1.86                     | 0.57              |
| 7:K:93:ILE:HG21   | 7:K:113:LEU:HD11  | 1.87                     | 0.57              |
| 16:Y:-80:DG:H2''  | 16:Y:-79:DT:C6    | 2.39                     | 0.57              |
| 2:B:75:SER:CB     | 2:B:86:ILE:HD11   | 2.35                     | 0.57              |
| 1:E:95:LYS:HZ2    | 1:E:95:LYS:HB3    | 1.70                     | 0.57              |
| 7:K:105:ILE:HG12  | 8:L:90:GLU:OE1    | 2.04                     | 0.57              |
| 13:V:189:GLU:CG   | 13:V:224:ARG:HD3  | 2.35                     | 0.57              |
| 3:C:130:ILE:HD12  | 3:G:130:ILE:HD12  | 1.86                     | 0.56              |
| 7:K:273:GLU:O     | 7:K:277:VAL:HG23  | 2.05                     | 0.56              |
| 13:V:272:ILE:HD12 | 14:W:187:LYS:HZ2  | 1.68                     | 0.56              |
| 16:Y:-42:DT:H2''  | 16:Y:-41:DA:H5'   | 1.87                     | 0.56              |
| 7:K:195:VAL:HG22  | 7:K:198:GLU:HG3   | 1.87                     | 0.56              |
| 9:M:416:LEU:HB2   | 9:M:433:ILE:HD11  | 1.86                     | 0.56              |
| 13:V:143:TYR:HA   | 13:V:147:LEU:HB2  | 1.87                     | 0.56              |
| 13:V:268:LEU:HD22 | 14:W:191:SER:OG   | 2.04                     | 0.56              |
| 15:X:8:DT:H2''    | 15:X:9:DA:H8      | 1.69                     | 0.56              |
| 5:I:125:PRO:HD2   | 13:V:222:HIS:CE1  | 2.40                     | 0.56              |
| 5:I:210:GLU:O     | 5:I:214:GLN:HG3   | 2.04                     | 0.56              |
| 5:I:921:ILE:HG22  | 5:I:1985:ALA:CB   | 2.19                     | 0.56              |
| 5:I:1992:ALA:HB2  | 10:N:201:LYS:HZ2  | 1.68                     | 0.56              |
| 7:K:205:VAL:HG11  | 7:K:269:ARG:CZ    | 2.35                     | 0.56              |
| 7:K:311:PRO:HA    | 7:K:314:PHE:CE2   | 2.40                     | 0.56              |
| 13:V:233:LEU:N    | 13:V:233:LEU:HD23 | 2.20                     | 0.56              |
| 13:V:262:GLU:HG3  | 14:W:202:LYS:CE   | 2.36                     | 0.56              |
| 16:Y:-56:DA:H2''  | 16:Y:-55:DC:C5    | 2.40                     | 0.56              |
| 1:A:35:LEU:HD11   | 1:A:52:LEU:HD23   | 1.88                     | 0.56              |
| 1:E:20:ARG:HG3    | 2:F:121:SER:CB    | 2.35                     | 0.56              |
| 7:K:36:ARG:NH2    | 7:K:37:LEU:HG     | 2.20                     | 0.56              |
| 7:K:232:VAL:HG22  | 7:K:233:MET:N     | 2.20                     | 0.56              |
| 13:V:206:ARG:C    | 13:V:209:PRO:HD2  | 2.30                     | 0.56              |
| 13:V:264:ARG:NH1  | 14:W:194:ILE:HG21 | 2.21                     | 0.56              |
| 13:V:265:SER:OG   | 14:W:198:LYS:HD3  | 2.06                     | 0.56              |
| 1:A:56:LEU:HD11   | 2:B:67:PHE:HD2    | 1.70                     | 0.56              |
| 1:E:85:LEU:HD22   | 1:E:108:LEU:HD23  | 1.87                     | 0.56              |
| 4:H:79:LYS:HB3    | 4:H:79:LYS:NZ     | 2.21                     | 0.56              |
| 7:K:13:ALA:HB3    | 7:K:25:ILE:HG12   | 1.87                     | 0.56              |
| 7:K:176:GLY:H     | 7:K:179:LEU:HD13  | 1.71                     | 0.56              |
| 14:W:137:GLU:HG2  | 14:W:170:THR:HB   | 1.88                     | 0.56              |
| 15:X:137:DG:H2''  | 15:X:138:DA:C8    | 2.41                     | 0.56              |
| 1:A:18:ARG:HH22   | 1:A:36:ARG:HH12   | 1.54                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:111:GLY:O     | 2:F:115:VAL:HG23  | 2.06                     | 0.56              |
| 7:K:81:LYS:HD2    | 7:K:82:GLU:N      | 2.21                     | 0.56              |
| 7:K:113:LEU:HA    | 7:K:117:TYR:HD2   | 1.70                     | 0.56              |
| 7:K:306:PRO:HB3   | 7:K:308:GLU:OE2   | 2.05                     | 0.56              |
| 13:V:156:GLU:OE1  | 13:V:183:PHE:CD2  | 2.59                     | 0.56              |
| 13:V:255:GLU:HA   | 13:V:259:LYS:HE2  | 1.86                     | 0.56              |
| 16:Y:-56:DA:H2''  | 16:Y:-55:DC:C6    | 2.40                     | 0.56              |
| 1:A:57:GLU:OE2    | 8:L:9:ARG:NH2     | 2.39                     | 0.56              |
| 11:U:117:GLU:CD   | 13:V:114:TRP:HE1  | 2.14                     | 0.56              |
| 1:E:85:LEU:HD22   | 1:E:108:LEU:CD2   | 2.36                     | 0.56              |
| 13:V:50:PRO:O     | 13:V:51:GLU:HG3   | 2.06                     | 0.56              |
| 7:K:67:ASN:C      | 7:K:69:ASP:H      | 2.14                     | 0.56              |
| 9:M:180:LEU:HD21  | 9:M:193:ILE:HD11  | 1.88                     | 0.56              |
| 9:M:317:ARG:CD    | 10:R:104:ALA:HB2  | 2.36                     | 0.56              |
| 15:X:125:DC:H2''  | 15:X:126:DC:H5'   | 1.88                     | 0.56              |
| 1:A:33:ARG:HH22   | 2:B:32:GLU:CD     | 2.13                     | 0.56              |
| 1:A:56:LEU:HD11   | 2:B:67:PHE:HB2    | 1.88                     | 0.56              |
| 2:B:28:ARG:HH12   | 16:Y:-21:DG:P     | 2.29                     | 0.56              |
| 4:H:97:LEU:HD11   | 4:H:100:PHE:HD1   | 1.71                     | 0.56              |
| 5:I:118:PHE:CG    | 13:V:247:LEU:HD13 | 2.40                     | 0.56              |
| 7:K:13:ALA:O      | 7:K:15:ILE:N      | 2.39                     | 0.56              |
| 7:K:183:HIS:O     | 7:K:187:ILE:HG12  | 2.05                     | 0.56              |
| 7:K:237:VAL:CG1   | 7:K:250:LYS:HE2   | 2.35                     | 0.56              |
| 7:K:337:VAL:O     | 7:K:341:THR:HG23  | 2.06                     | 0.56              |
| 9:M:416:LEU:HD22  | 9:M:433:ILE:CG1   | 2.36                     | 0.56              |
| 12:T:338:ILE:HD11 | 13:V:230:LEU:HD22 | 1.87                     | 0.56              |
| 5:I:167:ARG:HG2   | 15:X:31:DG:H5''   | 1.88                     | 0.55              |
| 7:K:133:HIS:O     | 7:K:137:ARG:HG3   | 2.06                     | 0.55              |
| 7:K:324:SER:HB2   | 7:K:351:LEU:HD11  | 1.88                     | 0.55              |
| 13:V:128:ARG:HG3  | 13:V:129:PHE:CD1  | 2.41                     | 0.55              |
| 13:V:143:TYR:CE1  | 13:V:154:LYS:HG3  | 2.40                     | 0.55              |
| 1:A:55:VAL:HG13   | 2:B:107:ALA:CB    | 2.34                     | 0.55              |
| 2:F:39:TYR:CZ     | 2:F:43:LYS:HE3    | 2.41                     | 0.55              |
| 7:K:62:LYS:HD2    | 7:K:172:ARG:HH12  | 1.71                     | 0.55              |
| 7:K:377:VAL:HG22  | 7:K:389:VAL:HG22  | 1.88                     | 0.55              |
| 10:N:39:PRO:HD3   | 10:N:54:ARG:HB2   | 1.88                     | 0.55              |
| 13:V:250:GLU:OE2  | 13:V:253:LYS:HD3  | 2.05                     | 0.55              |
| 13:V:261:ARG:HA   | 14:W:198:LYS:CE   | 2.37                     | 0.55              |
| 16:Y:-21:DG:H2'   | 16:Y:-20:DT:C7    | 2.33                     | 0.55              |
| 3:C:96:CYS:SG     | 4:D:62:LEU:HD21   | 2.46                     | 0.55              |
| 4:H:92:ARG:HB3    | 4:H:92:ARG:CZ     | 2.37                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 15:X:8:DT:H2''   | 15:X:9:DA:C8     | 2.42                     | 0.55              |
| 15:X:119:DG:H1'  | 15:X:120:DA:C8   | 2.42                     | 0.55              |
| 5:I:814:MET:HE1  | 5:I:822:ASN:HA   | 1.87                     | 0.55              |
| 16:Y:-77:DC:H2'' | 16:Y:-76:DG:C8   | 2.41                     | 0.55              |
| 2:F:99:LEU:HB2   | 2:F:104:ALA:CB   | 2.36                     | 0.55              |
| 7:K:1:MET:HE3    | 7:K:92:ASN:ND2   | 2.22                     | 0.55              |
| 7:K:159:PRO:HB3  | 7:K:313:PHE:HZ   | 1.72                     | 0.55              |
| 15:X:110:DC:H2'' | 15:X:111:DG:C8   | 2.42                     | 0.55              |
| 1:A:110:PRO:HA   | 3:C:55:GLN:OE1   | 2.06                     | 0.55              |
| 7:K:72:ARG:NH1   | 7:K:117:TYR:OH   | 2.39                     | 0.55              |
| 13:V:229:GLN:OE1 | 13:V:229:GLN:N   | 2.38                     | 0.55              |
| 16:Y:-110:DG:H4' | 16:Y:-110:DG:OP1 | 2.06                     | 0.55              |
| 1:A:85:GLN:O     | 1:A:89:ARG:HG2   | 2.07                     | 0.55              |
| 2:B:73:GLU:OE1   | 2:B:73:GLU:HA    | 2.07                     | 0.55              |
| 5:I:1914:LEU:CD1 | 9:M:282:VAL:HB   | 2.36                     | 0.55              |
| 13:V:96:LYS:N    | 13:V:114:TRP:HZ3 | 2.05                     | 0.55              |
| 15:X:51:DG:H1'   | 15:X:52:DG:C5'   | 2.31                     | 0.55              |
| 15:X:141:DC:H6   | 15:X:141:DC:H5'  | 1.71                     | 0.55              |
| 1:A:55:VAL:CG1   | 2:B:107:ALA:HB1  | 2.37                     | 0.55              |
| 4:D:23:ARG:NH2   | 14:W:81:VAL:CG1  | 2.63                     | 0.55              |
| 7:K:29:GLN:HB3   | 7:K:39:THR:HG22  | 1.88                     | 0.55              |
| 7:K:122:VAL:C    | 7:K:123:LEU:HD23 | 2.32                     | 0.55              |
| 7:K:128:GLY:O    | 7:K:147:ILE:HG13 | 2.06                     | 0.55              |
| 7:K:223:ALA:HA   | 7:K:230:ASN:O    | 2.06                     | 0.55              |
| 11:U:257:CYS:HB3 | 11:U:258:PRO:CD  | 2.37                     | 0.55              |
| 13:V:255:GLU:C   | 13:V:259:LYS:HE2 | 2.32                     | 0.55              |
| 16:Y:-24:DC:H2'' | 16:Y:-23:DA:C8   | 2.41                     | 0.55              |
| 4:D:75:HIS:CD2   | 2:F:89:ARG:HG2   | 2.42                     | 0.55              |
| 7:K:56:TYR:C     | 8:L:39:ASN:ND2   | 2.65                     | 0.55              |
| 7:K:237:VAL:HG12 | 7:K:267:ILE:HG22 | 1.89                     | 0.55              |
| 16:Y:-78:DA:H2'' | 16:Y:-77:DC:C6   | 2.41                     | 0.55              |
| 5:I:128:PRO:CB   | 13:V:216:PRO:HG2 | 2.37                     | 0.55              |
| 5:I:670:HIS:CD2  | 5:I:742:TYR:HD2  | 2.21                     | 0.55              |
| 7:K:75:TRP:HB3   | 7:K:79:PHE:CZ    | 2.42                     | 0.55              |
| 7:K:78:LEU:O     | 7:K:84:TYR:HB2   | 2.07                     | 0.55              |
| 7:K:292:MET:HE2  | 8:L:106:ALA:CB   | 2.37                     | 0.55              |
| 15:X:12:DT:H2''  | 15:X:13:DA:C8    | 2.42                     | 0.55              |
| 4:H:73:THR:OG1   | 4:H:85:ASP:OD2   | 2.18                     | 0.54              |
| 7:K:180:LEU:HB3  | 7:K:277:VAL:HG12 | 1.89                     | 0.54              |
| 5:I:921:ILE:CG2  | 5:I:1985:ALA:HB1 | 2.20                     | 0.54              |
| 7:K:376:VAL:CG1  | 7:K:377:VAL:N    | 2.67                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 15:X:4:DG:H2''    | 15:X:5:DA:H5''   | 1.89                     | 0.54              |
| 15:X:35:DA:H4'    | 15:X:35:DA:OP1   | 2.07                     | 0.54              |
| 7:K:172:ARG:NH2   | 7:K:174:ASN:HD21 | 2.05                     | 0.54              |
| 11:U:117:GLU:OE1  | 13:V:114:TRP:NE1 | 2.39                     | 0.54              |
| 15:X:100:DG:H1'   | 15:X:101:DA:N7   | 2.22                     | 0.54              |
| 16:Y:-39:DT:H4'   | 16:Y:-39:DT:OP1  | 2.06                     | 0.54              |
| 1:A:25:GLN:N      | 8:L:9:ARG:HH22   | 2.04                     | 0.54              |
| 2:B:93:THR:HG21   | 4:H:75:HIS:CD2   | 2.42                     | 0.54              |
| 2:B:116:THR:HG22  | 13:V:57:VAL:HG13 | 1.90                     | 0.54              |
| 13:V:104:ALA:HB2  | 13:V:127:ALA:HB1 | 1.89                     | 0.54              |
| 15:X:120:DA:H2''  | 15:X:121:DG:C8   | 2.42                     | 0.54              |
| 1:A:66:LEU:CD1    | 1:A:94:LEU:HD12  | 2.38                     | 0.54              |
| 3:C:130:ILE:HG21  | 3:G:130:ILE:HB   | 1.89                     | 0.54              |
| 1:E:25:PHE:HB2    | 1:E:56:GLU:OE1   | 2.07                     | 0.54              |
| 7:K:110:ASN:HB2   | 7:K:387:HIS:CD2  | 2.42                     | 0.54              |
| 7:K:377:VAL:HG21  | 7:K:393:LYS:HG3  | 1.90                     | 0.54              |
| 9:M:26:LEU:CD1    | 9:M:50:GLY:HA3   | 2.35                     | 0.54              |
| 11:U:362:TYR:HE2  | 13:V:91:LYS:HD3  | 1.73                     | 0.54              |
| 13:V:54:HIS:O     | 13:V:58:TYR:HB3  | 2.07                     | 0.54              |
| 15:X:120:DA:C2'   | 15:X:121:DG:C8   | 2.91                     | 0.54              |
| 16:Y:-12:DA:H2''  | 16:Y:-11:DT:H5'  | 1.89                     | 0.54              |
| 3:G:83:ARG:O      | 4:H:80:THR:HA    | 2.08                     | 0.54              |
| 5:I:128:PRO:CG    | 13:V:218:PHE:HA  | 2.38                     | 0.54              |
| 5:I:633:TYR:HD1   | 5:I:742:TYR:HE1  | 1.56                     | 0.54              |
| 5:I:2072:LEU:HB3  | 5:I:2088:ARG:CD  | 2.29                     | 0.54              |
| 13:V:258:LYS:O    | 13:V:262:GLU:N   | 2.36                     | 0.54              |
| 1:A:51:TYR:CD1    | 2:B:91:ILE:HG22  | 2.42                     | 0.54              |
| 3:G:55:GLN:HG2    | 3:G:55:GLN:O     | 2.07                     | 0.54              |
| 5:I:236:ILE:HA    | 5:I:239:GLN:HE21 | 1.72                     | 0.54              |
| 5:I:2092:SER:HA   | 15:X:56:DT:H73   | 1.90                     | 0.54              |
| 7:K:99:TYR:CE2    | 7:K:158:VAL:HG21 | 2.43                     | 0.54              |
| 7:K:121:ALA:HA    | 7:K:378:THR:OG1  | 2.07                     | 0.54              |
| 7:K:176:GLY:O     | 7:K:180:LEU:HG   | 2.07                     | 0.54              |
| 13:V:236:ARG:NH2  | 13:V:241:VAL:HA  | 2.23                     | 0.54              |
| 13:V:272:ILE:HD13 | 14:W:191:SER:HB2 | 1.88                     | 0.54              |
| 15:X:36:DG:N2     | 16:Y:-35:DT:O2   | 2.41                     | 0.54              |
| 1:A:51:TYR:CE1    | 2:B:95:VAL:HG21  | 2.43                     | 0.54              |
| 13:V:206:ARG:O    | 13:V:209:PRO:HD2 | 2.08                     | 0.54              |
| 15:X:39:DA:H2''   | 15:X:40:DG:H8    | 1.73                     | 0.54              |
| 15:X:109:DA:H61   | 16:Y:-109:DT:H3  | 1.55                     | 0.54              |
| 1:A:30:ARG:NH1    | 2:B:33:SER:O     | 2.34                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:71:ALA:HA     | 1:A:83:HIS:CD2    | 2.42                     | 0.54              |
| 4:H:38:ALA:HB1    | 4:H:43:VAL:HB     | 1.90                     | 0.54              |
| 5:I:2087:LEU:HD11 | 5:I:2104:ARG:CZ   | 2.37                     | 0.54              |
| 7:K:222:ILE:HG22  | 7:K:230:ASN:HA    | 1.90                     | 0.54              |
| 15:X:7:DG:C1'     | 15:X:8:DT:H5''    | 2.38                     | 0.54              |
| 15:X:135:DG:H2''  | 15:X:136:DG:O5'   | 2.07                     | 0.54              |
| 5:I:800:HIS:CG    | 5:I:801:ARG:H     | 2.26                     | 0.54              |
| 7:K:6:LEU:HD13    | 7:K:95:ILE:HG12   | 1.90                     | 0.54              |
| 7:K:112:ILE:HG23  | 7:K:116:GLU:CD    | 2.33                     | 0.54              |
| 7:K:225:LEU:HG    | 7:K:230:ASN:HB3   | 1.89                     | 0.54              |
| 7:K:294:ILE:N     | 7:K:295:PRO:HD2   | 2.23                     | 0.54              |
| 7:K:375:MET:O     | 7:K:376:VAL:CG1   | 2.54                     | 0.54              |
| 9:O:15:ILE:CG2    | 10:P:69:ALA:HB2   | 2.38                     | 0.54              |
| 15:X:57:DT:C6     | 15:X:57:DT:C5'    | 2.91                     | 0.54              |
| 13:V:225:ARG:O    | 13:V:229:GLN:OE1  | 2.25                     | 0.53              |
| 15:X:35:DA:H2''   | 15:X:36:DG:C8     | 2.43                     | 0.53              |
| 15:X:81:DG:C2'    | 15:X:82:DT:H71    | 2.38                     | 0.53              |
| 16:Y:-109:DT:H2'' | 16:Y:-108:DA:C5   | 2.43                     | 0.53              |
| 3:C:126:LEU:HD22  | 3:G:113:HIS:CG    | 2.43                     | 0.53              |
| 1:E:78:ILE:HG13   | 2:F:49:THR:CG2    | 2.38                     | 0.53              |
| 4:H:97:LEU:HD11   | 4:H:100:PHE:CE1   | 2.43                     | 0.53              |
| 7:K:62:LYS:HD2    | 7:K:172:ARG:HH22  | 1.72                     | 0.53              |
| 7:K:120:GLN:C     | 7:K:378:THR:CG2   | 2.81                     | 0.53              |
| 10:N:90:MET:HE1   | 10:N:325:ILE:HD12 | 1.90                     | 0.53              |
| 13:V:247:LEU:HD12 | 13:V:248:LEU:HD23 | 1.89                     | 0.53              |
| 13:V:258:LYS:CE   | 13:V:259:LYS:HG3  | 2.37                     | 0.53              |
| 15:X:75:DG:H2''   | 15:X:76:DC:C6     | 2.43                     | 0.53              |
| 16:Y:-60:DT:H71   | 16:Y:-60:DT:OP2   | 2.08                     | 0.53              |
| 3:C:47:ALA:O      | 3:C:51:ILE:HG13   | 2.08                     | 0.53              |
| 5:I:846:GLU:CG    | 5:I:848:GLN:HG2   | 2.36                     | 0.53              |
| 7:K:279:GLU:O     | 7:K:283:ASN:N     | 2.37                     | 0.53              |
| 13:V:251:LEU:O    | 13:V:255:GLU:HB2  | 2.09                     | 0.53              |
| 13:V:266:GLN:HA   | 13:V:266:GLN:NE2  | 2.23                     | 0.53              |
| 16:Y:-91:DC:H1'   | 16:Y:-90:DT:H5'   | 1.90                     | 0.53              |
| 16:Y:-13:DT:H2''  | 16:Y:-12:DA:H5'   | 1.89                     | 0.53              |
| 1:A:13:ALA:N      | 5:I:164:LYS:HB2   | 2.23                     | 0.53              |
| 1:A:116:LEU:HD22  | 3:C:117:VAL:HG13  | 1.90                     | 0.53              |
| 2:B:87:THR:O      | 2:B:91:ILE:HG12   | 2.07                     | 0.53              |
| 4:D:23:ARG:HH21   | 14:W:81:VAL:HG13  | 1.71                     | 0.53              |
| 1:E:42:ARG:NH1    | 15:X:112:DA:H5'   | 2.23                     | 0.53              |
| 5:I:128:PRO:HG3   | 13:V:216:PRO:O    | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:V:233:LEU:CA   | 13:V:236:ARG:HD3  | 2.27                     | 0.53              |
| 13:V:265:SER:OG   | 14:W:198:LYS:CD   | 2.56                     | 0.53              |
| 15:X:141:DC:C5'   | 15:X:141:DC:C6    | 2.92                     | 0.53              |
| 3:C:49:ARG:HD3    | 15:X:7:DG:OP1     | 2.09                     | 0.53              |
| 1:E:99:ARG:O      | 4:H:96:THR:HB     | 2.08                     | 0.53              |
| 7:K:50:ASP:OD1    | 7:K:52:SER:HB2    | 2.08                     | 0.53              |
| 7:K:72:ARG:HA     | 7:K:72:ARG:HH11   | 1.72                     | 0.53              |
| 7:K:241:PHE:HA    | 7:K:244:ILE:O     | 2.09                     | 0.53              |
| 1:A:26:PHE:HE2    | 2:B:63:VAL:CG1    | 2.21                     | 0.53              |
| 2:B:39:TYR:CE1    | 2:B:43:LYS:HE3    | 2.43                     | 0.53              |
| 5:I:667:TRP:CZ2   | 5:I:719:HIS:CE1   | 2.97                     | 0.53              |
| 5:I:969:LEU:CB    | 10:R:225:VAL:HA   | 2.38                     | 0.53              |
| 9:M:113:MET:CG    | 9:M:276:ARG:HH12  | 2.18                     | 0.53              |
| 13:V:202:LEU:HD13 | 13:V:206:ARG:HH22 | 1.72                     | 0.53              |
| 1:A:32:HIS:CA     | 1:A:49:PRO:HB3    | 2.39                     | 0.53              |
| 2:B:65:ASP:OD2    | 4:D:98:TYR:OH     | 2.26                     | 0.53              |
| 5:I:649:LYS:NZ    | 19:I:3303:BEF:F3  | 2.31                     | 0.53              |
| 5:I:1972:ILE:HG21 | 10:P:242:VAL:HG11 | 1.91                     | 0.53              |
| 7:K:133:HIS:NE2   | 7:K:362:GLY:O     | 2.42                     | 0.53              |
| 7:K:221:ASP:HA    | 7:K:224:LYS:NZ    | 2.24                     | 0.53              |
| 15:X:117:DT:H2''  | 15:X:118:DT:C6    | 2.44                     | 0.53              |
| 1:A:71:ALA:HA     | 1:A:83:HIS:NE2    | 2.24                     | 0.53              |
| 7:K:164:LYS:HZ1   | 7:K:166:LYS:HA    | 1.74                     | 0.53              |
| 10:N:59:VAL:HG21  | 10:N:325:ILE:HD11 | 1.91                     | 0.53              |
| 13:V:244:GLU:HA   | 13:V:247:LEU:HD21 | 1.90                     | 0.53              |
| 13:V:261:ARG:CB   | 14:W:198:LYS:HG2  | 2.39                     | 0.53              |
| 13:V:262:GLU:HG3  | 14:W:202:LYS:HG3  | 1.90                     | 0.53              |
| 1:A:33:ARG:O      | 1:A:36:ARG:HG3    | 2.08                     | 0.53              |
| 1:A:39:ASN:ND2    | 1:E:40:ALA:HA     | 2.24                     | 0.53              |
| 5:I:2088:ARG:HA   | 5:I:2115:ILE:O    | 2.08                     | 0.53              |
| 7:K:333:VAL:O     | 7:K:337:VAL:HG13  | 2.09                     | 0.53              |
| 16:Y:-116:DT:H5'  | 16:Y:-116:DT:H6   | 1.73                     | 0.53              |
| 16:Y:-85:DC:H1'   | 16:Y:-84:DG:C8    | 2.44                     | 0.53              |
| 16:Y:-41:DA:H2''  | 16:Y:-40:DC:C6    | 2.44                     | 0.53              |
| 1:A:51:TYR:CZ     | 2:B:92:GLN:HA     | 2.44                     | 0.53              |
| 3:C:113:HIS:NE2   | 3:G:110:CYS:O     | 2.42                     | 0.53              |
| 1:E:35:ARG:HB3    | 1:E:43:VAL:HG23   | 1.90                     | 0.53              |
| 5:I:895:MET:HE1   | 15:X:52:DG:H5''   | 1.90                     | 0.53              |
| 16:Y:-25:DG:H1'   | 16:Y:-24:DC:C5    | 2.44                     | 0.53              |
| 4:D:45:ARG:NH2    | 15:X:80:DC:O4'    | 2.42                     | 0.52              |
| 5:I:726:LYS:NZ    | 15:X:55:DG:H1'    | 2.25                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:X:59:DA:H2''   | 15:X:60:DA:OP2    | 2.08                     | 0.52              |
| 1:A:52:LEU:HD11   | 2:B:67:PHE:HA     | 1.90                     | 0.52              |
| 2:B:116:THR:HG22  | 13:V:57:VAL:CG1   | 2.40                     | 0.52              |
| 4:H:46:ILE:CG2    | 4:H:50:ILE:HG21   | 2.35                     | 0.52              |
| 7:K:88:PHE:CB     | 7:K:119:PHE:HD2   | 2.22                     | 0.52              |
| 7:K:191:ARG:NH1   | 7:K:273:GLU:OE1   | 2.42                     | 0.52              |
| 7:K:233:MET:HG2   | 7:K:252:ARG:HG3   | 1.91                     | 0.52              |
| 7:K:357:THR:O     | 7:K:361:GLU:HG3   | 2.09                     | 0.52              |
| 5:I:943:MET:HA    | 5:I:943:MET:HE2   | 1.90                     | 0.52              |
| 5:I:2063:LEU:CD1  | 5:I:2127:LEU:HD23 | 2.38                     | 0.52              |
| 5:I:2098:ARG:NH1  | 15:X:56:DT:OP2    | 2.40                     | 0.52              |
| 16:Y:-108:DA:H2'' | 16:Y:-107:DG:O5'  | 2.09                     | 0.52              |
| 1:E:17:ARG:N      | 16:Y:-116:DT:OP1  | 2.39                     | 0.52              |
| 13:V:91:LYS:HZ2   | 13:V:91:LYS:HB3   | 1.74                     | 0.52              |
| 13:V:96:LYS:HD3   | 13:V:97:TRP:O     | 2.09                     | 0.52              |
| 13:V:182:GLN:HB2  | 13:V:183:PHE:CD1  | 2.45                     | 0.52              |
| 13:V:189:GLU:HG3  | 13:V:224:ARG:HD3  | 1.91                     | 0.52              |
| 16:Y:-115:DT:H2'' | 16:Y:-114:DG:C8   | 2.44                     | 0.52              |
| 1:E:25:PHE:N      | 1:E:56:GLU:OE1    | 2.43                     | 0.52              |
| 7:K:107:GLU:HG3   | 7:K:108:SER:N     | 2.25                     | 0.52              |
| 7:K:338:ARG:HB2   | 7:K:347:VAL:HG11  | 1.90                     | 0.52              |
| 1:A:66:LEU:HB2    | 1:A:87:ALA:HB1    | 1.91                     | 0.52              |
| 5:I:1992:ALA:HB2  | 10:N:201:LYS:HZ3  | 1.75                     | 0.52              |
| 7:K:235:ASP:CG    | 7:K:255:MET:HG2   | 2.34                     | 0.52              |
| 15:X:49:DT:H2'    | 15:X:50:DT:H71    | 1.92                     | 0.52              |
| 16:Y:-25:DG:H4'   | 16:Y:-24:DC:OP1   | 2.10                     | 0.52              |
| 7:K:287:ILE:HG23  | 8:L:35:LEU:CD1    | 2.38                     | 0.52              |
| 3:C:42:ARG:NH2    | 16:Y:-78:DA:O5'   | 2.41                     | 0.52              |
| 5:I:888:MET:SD    | 15:X:51:DG:N1     | 2.82                     | 0.52              |
| 7:K:377:VAL:HG23  | 7:K:393:LYS:NZ    | 2.25                     | 0.52              |
| 9:M:36:ALA:O      | 9:M:38:GLY:N      | 2.42                     | 0.52              |
| 13:V:261:ARG:O    | 14:W:198:LYS:CE   | 2.56                     | 0.52              |
| 2:B:34:TYR:N      | 2:B:60:ASN:HD21   | 2.04                     | 0.52              |
| 3:C:103:LEU:HD11  | 3:C:128:ARG:HG2   | 1.92                     | 0.52              |
| 7:K:93:ILE:CG2    | 7:K:113:LEU:HD11  | 2.40                     | 0.52              |
| 7:K:157:ILE:O     | 7:K:170:ILE:HA    | 2.09                     | 0.52              |
| 7:K:376:VAL:O     | 7:K:377:VAL:CB    | 2.58                     | 0.52              |
| 15:X:66:DG:H2''   | 15:X:67:DG:N7     | 2.25                     | 0.52              |
| 1:E:101:THR:N     | 4:H:96:THR:O      | 2.32                     | 0.52              |
| 9:M:271:ILE:HD12  | 9:M:271:ILE:N     | 2.25                     | 0.52              |
| 9:O:447:LEU:HD11  | 10:P:344:HIS:CE1  | 2.44                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:V:98:MET:HB3   | 13:V:120:GLU:OE2  | 2.09                     | 0.52              |
| 13:V:187:SER:N    | 13:V:190:ASP:OD2  | 2.43                     | 0.52              |
| 15:X:105:DG:H1'   | 15:X:106:DT:H5'   | 1.91                     | 0.52              |
| 3:G:103:LEU:HD11  | 3:G:128:ARG:HG2   | 1.92                     | 0.51              |
| 13:V:147:LEU:HD12 | 13:V:198:ILE:HG12 | 1.92                     | 0.51              |
| 13:V:219:ASP:OD1  | 13:V:223:GLU:N    | 2.43                     | 0.51              |
| 16:Y:-13:DT:H2''  | 16:Y:-12:DA:C5'   | 2.41                     | 0.51              |
| 3:C:120:MET:C     | 4:D:50:ILE:HD11   | 2.35                     | 0.51              |
| 3:C:128:ARG:HD2   | 3:C:133:GLU:CD    | 2.35                     | 0.51              |
| 7:K:76:ASP:O      | 7:K:80:GLY:N      | 2.43                     | 0.51              |
| 7:K:119:PHE:O     | 7:K:120:GLN:O     | 2.28                     | 0.51              |
| 7:K:233:MET:HG2   | 7:K:252:ARG:HD2   | 1.91                     | 0.51              |
| 13:V:201:LYS:O    | 13:V:205:VAL:HG13 | 2.10                     | 0.51              |
| 15:X:59:DA:C2'    | 15:X:60:DA:H5''   | 2.39                     | 0.51              |
| 15:X:76:DC:H2'    | 15:X:76:DC:OP2    | 2.11                     | 0.51              |
| 16:Y:-12:DA:H1'   | 16:Y:-11:DT:H5''  | 1.92                     | 0.51              |
| 1:A:33:ARG:HB2    | 1:A:36:ARG:NH2    | 2.24                     | 0.51              |
| 1:A:60:THR:CG2    | 2:B:63:VAL:HG22   | 2.40                     | 0.51              |
| 7:K:174:ASN:HB2   | 7:K:291:GLU:OE1   | 2.10                     | 0.51              |
| 7:K:282:PHE:CZ    | 7:K:333:VAL:HG23  | 2.46                     | 0.51              |
| 7:K:385:ASN:OD1   | 7:K:385:ASN:N     | 2.43                     | 0.51              |
| 9:M:274:LYS:O     | 9:M:278:GLU:HG2   | 2.10                     | 0.51              |
| 15:X:68:DG:H1'    | 15:X:69:DG:C8     | 2.45                     | 0.51              |
| 1:A:33:ARG:HG3    | 15:X:28:DG:OP2    | 2.09                     | 0.51              |
| 1:A:84:LEU:O      | 1:A:88:ILE:HD12   | 2.10                     | 0.51              |
| 7:K:380:GLU:OE1   | 7:K:381:ASP:N     | 2.40                     | 0.51              |
| 13:V:98:MET:CE    | 13:V:120:GLU:HB2  | 2.41                     | 0.51              |
| 13:V:138:TYR:HB3  | 13:V:202:LEU:HD21 | 1.93                     | 0.51              |
| 3:C:74:ILE:HG23   | 4:D:63:GLU:HG2    | 1.93                     | 0.51              |
| 1:E:87:ILE:HD13   | 1:E:97:LEU:HD12   | 1.92                     | 0.51              |
| 7:K:66:VAL:C      | 7:K:68:TRP:H      | 2.18                     | 0.51              |
| 7:K:112:ILE:O     | 7:K:116:GLU:HB2   | 2.11                     | 0.51              |
| 7:K:280:ILE:HG12  | 7:K:287:ILE:HG12  | 1.92                     | 0.51              |
| 7:K:285:SER:HA    | 7:K:289:ILE:O     | 2.11                     | 0.51              |
| 15:X:111:DG:C2    | 16:Y:-110:DG:N2   | 2.78                     | 0.51              |
| 16:Y:-9:DT:H2''   | 16:Y:-8:DA:C8     | 2.45                     | 0.51              |
| 1:A:58:TYR:OH     | 1:A:62:GLU:OE2    | 2.25                     | 0.51              |
| 2:B:77:LEU:CD2    | 2:B:93:THR:HG23   | 2.41                     | 0.51              |
| 2:B:122:LYS:HB3   | 8:L:2:VAL:HG12    | 1.90                     | 0.51              |
| 1:E:81:ARG:HG2    | 3:G:58:THR:HG23   | 1.93                     | 0.51              |
| 4:H:92:ARG:HB3    | 4:H:92:ARG:NH1    | 2.26                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:K:13:ALA:HB3    | 7:K:25:ILE:CG1    | 2.41                     | 0.51              |
| 7:K:106:GLN:CB    | 7:K:124:ARG:HH22  | 2.18                     | 0.51              |
| 13:V:92:VAL:O     | 13:V:92:VAL:HG22  | 2.10                     | 0.51              |
| 15:X:138:DA:H2''  | 15:X:139:DT:C7    | 2.40                     | 0.51              |
| 1:E:65:LEU:CB     | 1:E:86:ALA:HB1    | 2.39                     | 0.51              |
| 3:G:41:TYR:CD1    | 3:G:45:THR:HG21   | 2.45                     | 0.51              |
| 5:I:895:MET:CE    | 15:X:52:DG:H4'    | 2.40                     | 0.51              |
| 5:I:1886:LEU:HB2  | 5:I:1889:LEU:HB2  | 1.93                     | 0.51              |
| 12:T:340:ILE:HD13 | 13:V:172:VAL:HG11 | 1.92                     | 0.51              |
| 13:V:225:ARG:O    | 13:V:228:GLU:N    | 2.43                     | 0.51              |
| 3:C:121:PRO:HA    | 4:D:50:ILE:CD1    | 2.41                     | 0.51              |
| 5:I:918:THR:O     | 5:I:921:ILE:HG23  | 2.10                     | 0.51              |
| 7:K:234:ILE:CD1   | 7:K:271:ALA:HA    | 2.32                     | 0.51              |
| 9:O:235:ILE:HG23  | 9:O:235:ILE:O     | 2.11                     | 0.51              |
| 11:U:101:HIS:CD2  | 11:U:101:HIS:N    | 2.78                     | 0.51              |
| 1:A:89:ARG:NH1    | 1:A:95:ASN:OD1    | 2.39                     | 0.51              |
| 5:I:619:ARG:NH1   | 17:I:3301:ADP:C6  | 2.79                     | 0.51              |
| 5:I:1954:ALA:CB   | 9:Q:124:ILE:HD11  | 2.41                     | 0.51              |
| 7:K:13:ALA:O      | 7:K:15:ILE:HG23   | 2.11                     | 0.51              |
| 7:K:171:ILE:HG22  | 7:K:173:ILE:HG12  | 1.92                     | 0.51              |
| 10:P:205:LEU:H    | 10:P:205:LEU:HD22 | 1.76                     | 0.51              |
| 15:X:10:DT:H2''   | 15:X:11:DA:OP2    | 2.10                     | 0.51              |
| 15:X:21:DC:H1'    | 15:X:22:DG:H5''   | 1.91                     | 0.51              |
| 15:X:47:DC:H2''   | 15:X:48:DC:C6     | 2.45                     | 0.51              |
| 15:X:57:DT:H6     | 15:X:57:DT:C5'    | 2.21                     | 0.51              |
| 3:C:96:CYS:HB3    | 4:D:58:LEU:HD11   | 1.92                     | 0.51              |
| 3:G:120:MET:HB2   | 3:G:121:PRO:HD2   | 1.91                     | 0.51              |
| 5:I:126:LYS:HE2   | 13:V:216:PRO:O    | 2.11                     | 0.51              |
| 5:I:2071:MET:HE2  | 5:I:2136:TYR:CE1  | 2.46                     | 0.51              |
| 9:M:313:THR:HG21  | 10:R:303:MET:CG   | 2.40                     | 0.51              |
| 1:A:67:ALA:HA     | 1:A:83:HIS:O      | 2.11                     | 0.50              |
| 7:K:38:LYS:HD2    | 7:K:40:PHE:CG     | 2.46                     | 0.50              |
| 7:K:232:VAL:HG13  | 7:K:233:MET:H     | 1.75                     | 0.50              |
| 13:V:212:ASP:C    | 13:V:214:LYS:H    | 2.19                     | 0.50              |
| 15:X:22:DG:H2''   | 15:X:23:DT:C5'    | 2.17                     | 0.50              |
| 15:X:103:DC:C6    | 15:X:104:DT:H72   | 2.46                     | 0.50              |
| 16:Y:-11:DT:H2''  | 16:Y:-10:DA:H5'   | 1.92                     | 0.50              |
| 16:Y:-11:DT:H1'   | 16:Y:-10:DA:H5''  | 1.91                     | 0.50              |
| 1:E:57:TYR:CD1    | 2:F:110:GLU:HG3   | 2.46                     | 0.50              |
| 1:E:71:ARG:HA     | 1:E:75:LYS:O      | 2.11                     | 0.50              |
| 3:G:116:ARG:HH21  | 3:G:122:LYS:HE3   | 1.76                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:I:180:GLU:N     | 5:I:180:GLU:OE1  | 2.43                     | 0.50              |
| 5:I:621:TYR:OH    | 5:I:846:GLU:OE1  | 2.28                     | 0.50              |
| 5:I:917:ILE:HD12  | 9:O:128:LYS:HZ1  | 1.75                     | 0.50              |
| 5:I:921:ILE:HD13  | 5:I:1986:PRO:HB2 | 1.92                     | 0.50              |
| 5:I:1941:PRO:HG2  | 5:I:1945:HIS:HD2 | 1.76                     | 0.50              |
| 9:O:401:THR:O     | 9:O:402:THR:HG23 | 2.11                     | 0.50              |
| 15:X:133:DC:H1'   | 15:X:134:DC:H5'  | 1.93                     | 0.50              |
| 1:E:100:VAL:HA    | 4:H:96:THR:O     | 2.12                     | 0.50              |
| 5:I:1992:ALA:CB   | 10:N:201:LYS:HZ3 | 2.25                     | 0.50              |
| 7:K:1:MET:HE3     | 7:K:92:ASN:OD1   | 2.12                     | 0.50              |
| 7:K:237:VAL:CG1   | 7:K:267:ILE:HG22 | 2.40                     | 0.50              |
| 7:K:337:VAL:HG23  | 7:K:347:VAL:HG21 | 1.92                     | 0.50              |
| 9:M:310:GLU:HA    | 9:M:313:THR:HG22 | 1.93                     | 0.50              |
| 9:Q:255:ASP:O     | 9:Q:257:LEU:N    | 2.45                     | 0.50              |
| 9:Q:306:MET:HE2   | 10:R:307:GLU:HA  | 1.93                     | 0.50              |
| 16:Y:-138:DT:H2'' | 16:Y:-137:DC:C6  | 2.46                     | 0.50              |
| 5:I:895:MET:HE1   | 15:X:52:DG:H4'   | 1.93                     | 0.50              |
| 5:I:904:PRO:O     | 5:I:908:ASP:N    | 2.43                     | 0.50              |
| 7:K:88:PHE:O      | 7:K:119:PHE:HB2  | 2.11                     | 0.50              |
| 7:K:284:PRO:HG3   | 7:K:293:GLY:N    | 2.27                     | 0.50              |
| 13:V:226:ARG:HA   | 13:V:229:GLN:OE1 | 2.11                     | 0.50              |
| 15:X:70:DA:H8     | 15:X:70:DA:OP2   | 1.94                     | 0.50              |
| 1:E:74:LYS:HD3    | 6:J:151:ARG:CD   | 2.40                     | 0.50              |
| 1:E:81:ARG:NH2    | 1:E:107:VAL:O    | 2.43                     | 0.50              |
| 3:G:48:LEU:HD23   | 3:G:51:ILE:HD12  | 1.94                     | 0.50              |
| 7:K:89:LEU:HD13   | 7:K:89:LEU:N     | 2.26                     | 0.50              |
| 16:Y:-56:DA:H1'   | 16:Y:-55:DC:C6   | 2.46                     | 0.50              |
| 16:Y:-24:DC:H1'   | 16:Y:-23:DA:C8   | 2.46                     | 0.50              |
| 16:Y:-23:DA:H2'   | 16:Y:-22:DC:C5   | 2.46                     | 0.50              |
| 3:G:61:LEU:H      | 3:G:97:GLU:CD    | 2.20                     | 0.50              |
| 7:K:310:GLN:O     | 7:K:313:PHE:HB2  | 2.11                     | 0.50              |
| 11:U:117:GLU:HB2  | 13:V:114:TRP:HE1 | 1.77                     | 0.50              |
| 16:Y:-84:DG:OP2   | 16:Y:-84:DG:H8   | 1.94                     | 0.50              |
| 3:C:46:VAL:HG22   | 3:C:49:ARG:HH21  | 1.77                     | 0.50              |
| 3:G:116:ARG:HH22  | 3:G:123:ASP:CG   | 2.19                     | 0.50              |
| 7:K:157:ILE:CG2   | 7:K:298:ILE:HA   | 2.42                     | 0.50              |
| 1:A:81:PRO:HB2    | 1:A:105:GLN:C    | 2.37                     | 0.50              |
| 7:K:79:PHE:HB3    | 7:K:88:PHE:CE1   | 2.47                     | 0.50              |
| 15:X:75:DG:H1     | 16:Y:-75:DC:N4   | 2.06                     | 0.50              |
| 1:E:64:GLU:HA     | 2:F:46:HIS:CE1   | 2.46                     | 0.50              |
| 5:I:726:LYS:HD2   | 15:X:56:DT:C4'   | 2.42                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:I:2060:HIS:CD2  | 5:I:2132:THR:HG21  | 2.39                     | 0.50              |
| 7:K:133:HIS:HE1   | 7:K:137:ARG:HD2    | 1.76                     | 0.50              |
| 7:K:160:TYR:CE1   | 7:K:165:LYS:HB2    | 2.47                     | 0.50              |
| 11:U:237:GLU:OE1  | 11:U:237:GLU:N     | 2.44                     | 0.50              |
| 13:V:56:GLU:H     | 13:V:56:GLU:CD     | 2.19                     | 0.50              |
| 13:V:169:LEU:HD21 | 13:V:195:TYR:CE2   | 2.47                     | 0.50              |
| 3:C:73:GLU:O      | 3:C:76:GLN:HB2     | 2.11                     | 0.49              |
| 1:E:70:ALA:O      | 1:E:75:LYS:HB2     | 2.12                     | 0.49              |
| 5:I:1914:LEU:CD2  | 9:M:285:LYS:HD2    | 2.42                     | 0.49              |
| 5:I:2072:LEU:HD13 | 5:I:2088:ARG:HH11  | 1.77                     | 0.49              |
| 7:K:233:MET:HG2   | 7:K:252:ARG:CG     | 2.42                     | 0.49              |
| 13:V:249:GLN:HG2  | 13:V:250:GLU:N     | 2.24                     | 0.49              |
| 13:V:258:LYS:C    | 13:V:261:ARG:H     | 2.20                     | 0.49              |
| 15:X:128:DC:H2''  | 15:X:129:DG:H5''   | 1.92                     | 0.49              |
| 16:Y:-125:DG:C2'  | 16:Y:-124:DC:H5''  | 2.36                     | 0.49              |
| 16:Y:-103:DG:OP1  | 16:Y:-103:DG:H4'   | 2.12                     | 0.49              |
| 1:A:33:ARG:HD2    | 1:A:37:LYS:HE2     | 1.94                     | 0.49              |
| 2:B:119:THR:HB    | 13:V:54:HIS:CD2    | 2.47                     | 0.49              |
| 7:K:175:VAL:HG21  | 7:K:289:ILE:HG21   | 1.94                     | 0.49              |
| 7:K:378:THR:HB    | 7:K:380:GLU:HG3    | 1.93                     | 0.49              |
| 9:M:113:MET:CG    | 9:M:276:ARG:NH1    | 2.56                     | 0.49              |
| 12:T:408:GLN:HA   | 13:V:105:ARG:HH11  | 1.76                     | 0.49              |
| 13:V:104:ALA:HB1  | 13:V:130:ASN:HD22  | 1.77                     | 0.49              |
| 15:X:11:DA:H2'    | 15:X:12:DT:H71     | 1.94                     | 0.49              |
| 16:Y:-133:DG:C2'  | 16:Y:-132:DT:H72   | 2.42                     | 0.49              |
| 16:Y:-75:DC:H1'   | 16:Y:-74:DG:H5'    | 1.94                     | 0.49              |
| 1:A:66:LEU:HD13   | 1:A:91:ASP:HB2     | 1.94                     | 0.49              |
| 5:I:112:GLU:OE1   | 13:V:247:LEU:CD2   | 2.60                     | 0.49              |
| 5:I:622:GLN:NE2   | 17:I:3301:ADP:HN61 | 2.11                     | 0.49              |
| 5:I:913:THR:HG23  | 5:I:2031:GLN:HB2   | 1.93                     | 0.49              |
| 5:I:2167:ILE:HD11 | 5:I:2177:LEU:HD22  | 1.93                     | 0.49              |
| 7:K:64:TYR:O      | 7:K:66:VAL:HG22    | 2.13                     | 0.49              |
| 7:K:121:ALA:CA    | 7:K:378:THR:OG1    | 2.60                     | 0.49              |
| 15:X:78:DT:H2''   | 15:X:79:DA:C8      | 2.46                     | 0.49              |
| 16:Y:-83:DC:H1'   | 16:Y:-82:DA:H5'    | 1.93                     | 0.49              |
| 2:B:38:VAL:HG11   | 2:B:59:MET:HG2     | 1.95                     | 0.49              |
| 3:C:127:ALA:O     | 3:G:130:ILE:HG21   | 2.13                     | 0.49              |
| 3:G:124:ILE:O     | 3:G:128:ARG:HG3    | 2.12                     | 0.49              |
| 5:I:888:MET:CE    | 15:X:51:DG:N1      | 2.76                     | 0.49              |
| 7:K:119:PHE:O     | 7:K:119:PHE:CD1    | 2.65                     | 0.49              |
| 7:K:156:HIS:NE2   | 7:K:172:ARG:HB2    | 2.28                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:K:234:ILE:HG13  | 7:K:271:ALA:HB2   | 1.94                     | 0.49              |
| 13:V:265:SER:HG   | 14:W:195:ALA:HA   | 1.76                     | 0.49              |
| 16:Y:-12:DA:H1'   | 16:Y:-11:DT:C5'   | 2.42                     | 0.49              |
| 3:C:76:GLN:OE1    | 3:C:76:GLN:HA     | 2.13                     | 0.49              |
| 3:C:127:ALA:HA    | 3:G:130:ILE:HG21  | 1.95                     | 0.49              |
| 5:I:2014:LEU:CD1  | 9:Q:256:ILE:HG13  | 2.33                     | 0.49              |
| 7:K:87:ASP:HB2    | 7:K:91:THR:HG21   | 1.93                     | 0.49              |
| 7:K:187:ILE:O     | 7:K:191:ARG:HG3   | 2.12                     | 0.49              |
| 8:L:27:ARG:HE     | 8:L:153:THR:HG21  | 1.65                     | 0.49              |
| 13:V:119:GLU:OE1  | 13:V:119:GLU:CA   | 2.59                     | 0.49              |
| 13:V:152:TRP:CZ3  | 13:V:194:ARG:HG2  | 2.47                     | 0.49              |
| 13:V:256:ALA:HB1  | 13:V:260:GLU:OE2  | 2.12                     | 0.49              |
| 16:Y:-119:DC:H1'  | 16:Y:-118:DA:O4'  | 2.13                     | 0.49              |
| 16:Y:-61:DT:H2''  | 16:Y:-60:DT:C5    | 2.48                     | 0.49              |
| 16:Y:-7:DC:H1'    | 16:Y:-6:DA:H5''   | 1.94                     | 0.49              |
| 16:Y:-1:DG:H2''   | 16:Y:0:DT:H5''    | 1.94                     | 0.49              |
| 3:C:128:ARG:HD2   | 3:C:133:GLU:OE1   | 2.12                     | 0.49              |
| 5:I:2014:LEU:HG   | 5:I:2017:ARG:CD   | 2.37                     | 0.49              |
| 7:K:64:TYR:HH     | 8:L:101:TYR:HE2   | 1.51                     | 0.49              |
| 7:K:239:PRO:HG3   | 7:K:247:GLY:N     | 2.28                     | 0.49              |
| 10:N:38:GLU:OE1   | 10:N:54:ARG:CZ    | 2.57                     | 0.49              |
| 2:F:99:LEU:HB2    | 2:F:104:ALA:CA    | 2.42                     | 0.49              |
| 3:G:94:GLU:HG3    | 4:H:100:PHE:HZ    | 1.78                     | 0.49              |
| 5:I:811:LEU:HA    | 5:I:814:MET:HG2   | 1.95                     | 0.49              |
| 10:N:52:ALA:CB    | 10:N:359:THR:HG22 | 2.41                     | 0.49              |
| 10:P:272:VAL:O    | 10:P:276:ILE:HG12 | 2.12                     | 0.49              |
| 13:V:98:MET:HB3   | 13:V:120:GLU:CD   | 2.38                     | 0.49              |
| 13:V:261:ARG:HB3  | 14:W:198:LYS:HG2  | 1.94                     | 0.49              |
| 16:Y:-146:DC:H2'' | 16:Y:-145:DT:H6   | 1.76                     | 0.49              |
| 2:B:77:LEU:HD13   | 4:H:72:TYR:CE1    | 2.47                     | 0.49              |
| 1:E:42:ARG:HB3    | 2:F:85:THR:CB     | 2.43                     | 0.49              |
| 3:G:118:THR:HG23  | 4:H:45:ARG:CB     | 2.42                     | 0.49              |
| 7:K:99:TYR:CZ     | 7:K:158:VAL:HG21  | 2.47                     | 0.49              |
| 15:X:39:DA:H2''   | 15:X:40:DG:C8     | 2.48                     | 0.49              |
| 16:Y:-142:DA:C1'  | 16:Y:-141:DG:H5'  | 2.42                     | 0.49              |
| 16:Y:-27:DA:H2''  | 16:Y:-26:DG:C8    | 2.47                     | 0.49              |
| 3:C:82:LEU:HD13   | 4:D:81:VAL:CG2    | 2.43                     | 0.49              |
| 3:G:61:LEU:HD22   | 4:H:36:ARG:HD2    | 1.95                     | 0.49              |
| 3:G:94:GLU:HG3    | 4:H:100:PHE:CZ    | 2.47                     | 0.49              |
| 7:K:237:VAL:HG22  | 7:K:250:LYS:HG3   | 1.95                     | 0.49              |
| 15:X:145:DA:H2''  | 15:X:146:DG:H5''  | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Y:-101:DT:C2'  | 16:Y:-100:DC:H5'  | 2.42                     | 0.49              |
| 16:Y:-49:DA:H2''  | 16:Y:-48:DG:C8    | 2.48                     | 0.49              |
| 16:Y:-22:DC:C2'   | 16:Y:-21:DG:C8    | 2.96                     | 0.49              |
| 1:A:48:ALA:HA     | 2:B:91:ILE:HG13   | 1.95                     | 0.49              |
| 1:E:73:ASN:HD22   | 1:E:73:ASN:C      | 2.20                     | 0.49              |
| 3:G:107:THR:HG21  | 3:G:124:ILE:CG1   | 2.43                     | 0.49              |
| 5:I:163:ARG:HA    | 5:I:166:VAL:HG22  | 1.95                     | 0.49              |
| 7:K:173:ILE:HG22  | 7:K:174:ASN:H     | 1.77                     | 0.49              |
| 7:K:179:LEU:H     | 7:K:179:LEU:HD12  | 1.77                     | 0.49              |
| 15:X:40:DG:H2'    | 15:X:41:DT:H71    | 1.94                     | 0.49              |
| 1:A:35:LEU:HD22   | 1:A:40:TYR:HD2    | 1.78                     | 0.48              |
| 2:B:75:SER:HA     | 2:B:86:ILE:CD1    | 2.43                     | 0.48              |
| 5:I:2014:LEU:HG   | 5:I:2017:ARG:HB2  | 1.94                     | 0.48              |
| 7:K:62:LYS:O      | 7:K:62:LYS:HD3    | 2.12                     | 0.48              |
| 7:K:78:LEU:HD23   | 7:K:83:MET:CE     | 2.43                     | 0.48              |
| 7:K:306:PRO:O     | 7:K:309:MET:N     | 2.43                     | 0.48              |
| 7:K:314:PHE:CZ    | 7:K:345:TYR:HB3   | 2.47                     | 0.48              |
| 15:X:2:DA:H2''    | 15:X:3:DG:C8      | 2.46                     | 0.48              |
| 16:Y:-19:DG:H2''  | 16:Y:-18:DT:H5''  | 1.95                     | 0.48              |
| 1:A:101:VAL:HG22  | 4:D:96:THR:HB     | 1.94                     | 0.48              |
| 2:B:89:ARG:NH2    | 4:H:75:HIS:HA     | 2.29                     | 0.48              |
| 3:C:128:ARG:HA    | 3:C:131:ARG:HD2   | 1.94                     | 0.48              |
| 5:I:102:HIS:CE1   | 13:V:253:LYS:HE2  | 2.48                     | 0.48              |
| 15:X:23:DT:H2''   | 15:X:24:DG:C8     | 2.48                     | 0.48              |
| 16:Y:-98:DA:C2'   | 16:Y:-97:DG:C8    | 2.95                     | 0.48              |
| 3:C:119:ILE:O     | 3:C:119:ILE:HG13  | 2.13                     | 0.48              |
| 5:I:949:ILE:HD12  | 9:M:249:ARG:C     | 2.37                     | 0.48              |
| 7:K:51:PRO:O      | 7:K:54:LEU:HG     | 2.14                     | 0.48              |
| 7:K:145:CYS:O     | 7:K:160:TYR:HB2   | 2.14                     | 0.48              |
| 7:K:152:TYR:CE2   | 7:K:178:LYS:HG2   | 2.48                     | 0.48              |
| 10:N:38:GLU:OE2   | 10:N:54:ARG:NH1   | 2.45                     | 0.48              |
| 9:O:306:MET:HE3   | 10:P:307:GLU:HA   | 1.95                     | 0.48              |
| 10:R:324:LEU:HD13 | 10:R:326:MET:HE3  | 1.96                     | 0.48              |
| 12:T:338:ILE:CD1  | 13:V:234:TYR:HB2  | 2.44                     | 0.48              |
| 13:V:184:LYS:HE2  | 13:V:186:ARG:NH2  | 2.28                     | 0.48              |
| 1:A:31:VAL:HG12   | 1:A:32:HIS:N      | 2.29                     | 0.48              |
| 2:B:99:LEU:HD23   | 2:B:99:LEU:N      | 2.28                     | 0.48              |
| 3:G:73:GLU:N      | 4:H:23:ARG:HH12   | 2.12                     | 0.48              |
| 5:I:106:ILE:CD1   | 13:V:254:ILE:HG22 | 2.43                     | 0.48              |
| 7:K:167:LYS:HZ2   | 7:K:170:ILE:HG21  | 1.78                     | 0.48              |
| 7:K:196:MET:HG3   | 8:L:41:GLN:HE22   | 1.79                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:K:292:MET:HE1   | 7:K:297:ALA:HB2   | 1.94                     | 0.48              |
| 13:V:245:GLU:O    | 13:V:248:LEU:HB2  | 2.14                     | 0.48              |
| 13:V:264:ARG:HH12 | 14:W:194:ILE:CD1  | 2.12                     | 0.48              |
| 3:G:111:ALA:HA    | 3:G:123:ASP:CG    | 2.37                     | 0.48              |
| 7:K:146:ILE:HG13  | 7:K:317:ILE:HA    | 1.94                     | 0.48              |
| 7:K:177:GLY:O     | 7:K:181:THR:OG1   | 2.32                     | 0.48              |
| 7:K:183:HIS:CD2   | 7:K:277:VAL:HG13  | 2.48                     | 0.48              |
| 7:K:294:ILE:O     | 7:K:298:ILE:HG13  | 2.13                     | 0.48              |
| 7:K:330:ARG:CG    | 7:K:351:LEU:HB2   | 2.43                     | 0.48              |
| 8:L:15:GLN:O      | 8:L:15:GLN:HG2    | 2.13                     | 0.48              |
| 13:V:196:TYR:HB3  | 13:V:217:VAL:HG13 | 1.95                     | 0.48              |
| 13:V:238:PRO:O    | 13:V:240:GLN:N    | 2.47                     | 0.48              |
| 13:V:245:GLU:OE2  | 13:V:246:TYR:HB2  | 2.13                     | 0.48              |
| 16:Y:-20:DT:H2''  | 16:Y:-19:DG:H8    | 1.79                     | 0.48              |
| 2:F:86:ILE:O      | 2:F:86:ILE:HG22   | 2.13                     | 0.48              |
| 2:F:110:GLU:HA    | 2:F:110:GLU:OE1   | 2.11                     | 0.48              |
| 3:G:82:LEU:CD1    | 4:H:70:VAL:HG13   | 2.42                     | 0.48              |
| 17:I:3301:ADP:O2B | 19:I:3303:BEF:F3  | 2.22                     | 0.48              |
| 7:K:15:ILE:CD1    | 7:K:78:LEU:HB3    | 2.44                     | 0.48              |
| 7:K:134:ARG:HD2   | 7:K:361:GLU:HB2   | 1.94                     | 0.48              |
| 7:K:376:VAL:C     | 7:K:393:LYS:HZ3   | 2.22                     | 0.48              |
| 8:L:27:ARG:HH21   | 8:L:153:THR:HG23  | 1.78                     | 0.48              |
| 11:U:117:GLU:HB2  | 13:V:114:TRP:NE1  | 2.28                     | 0.48              |
| 11:U:117:GLU:CB   | 13:V:114:TRP:HE1  | 2.27                     | 0.48              |
| 13:V:261:ARG:CA   | 14:W:198:LYS:HG2  | 2.43                     | 0.48              |
| 15:X:116:DA:H2'   | 15:X:117:DT:C6    | 2.48                     | 0.48              |
| 2:B:90:GLU:HG3    | 4:H:75:HIS:NE2    | 2.29                     | 0.48              |
| 2:B:112:THR:O     | 2:B:116:THR:HG23  | 2.14                     | 0.48              |
| 1:E:64:GLU:CB     | 2:F:45:VAL:HG11   | 2.37                     | 0.48              |
| 7:K:81:LYS:HB2    | 7:K:85:GLN:HE22   | 1.78                     | 0.48              |
| 7:K:314:PHE:HA    | 7:K:317:ILE:HG13  | 1.95                     | 0.48              |
| 15:X:128:DC:H6    | 15:X:128:DC:H5''  | 1.78                     | 0.48              |
| 5:I:1972:ILE:CG2  | 5:I:1976:PHE:CD2  | 2.74                     | 0.48              |
| 7:K:316:ASN:O     | 7:K:318:VAL:HG23  | 2.14                     | 0.48              |
| 16:Y:-130:DC:OP2  | 16:Y:-130:DC:H6   | 1.97                     | 0.48              |
| 16:Y:-42:DT:H2''  | 16:Y:-41:DA:C5'   | 2.44                     | 0.48              |
| 3:C:41:TYR:HB2    | 15:X:83:DG:P      | 2.54                     | 0.48              |
| 1:E:47:ALA:HB3    | 1:E:48:PRO:HD3    | 1.96                     | 0.48              |
| 5:I:125:PRO:HD2   | 13:V:222:HIS:NE2  | 2.29                     | 0.48              |
| 7:K:16:GLY:HA3    | 7:K:360:TRP:HE1   | 1.79                     | 0.48              |
| 7:K:88:PHE:O      | 7:K:119:PHE:CB    | 2.61                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:K:89:LEU:HD23   | 7:K:90:ASP:H      | 1.79                     | 0.48              |
| 7:K:97:GLU:HG3    | 7:K:126:ASN:HD22  | 1.77                     | 0.48              |
| 13:V:206:ARG:O    | 13:V:208:VAL:HG13 | 2.14                     | 0.48              |
| 16:Y:-54:DC:C2'   | 16:Y:-53:DG:C8    | 2.95                     | 0.48              |
| 1:E:118:LYS:HD2   | 1:E:118:LYS:C     | 2.39                     | 0.48              |
| 5:I:2000:ALA:HB3  | 5:I:2001:PRO:HD3  | 1.95                     | 0.48              |
| 7:K:56:TYR:CA     | 8:L:39:ASN:ND2    | 2.77                     | 0.48              |
| 7:K:229:GLU:HG2   | 7:K:230:ASN:N     | 2.29                     | 0.48              |
| 7:K:277:VAL:HB    | 7:K:278:PRO:CD    | 2.41                     | 0.48              |
| 7:K:292:MET:HB2   | 7:K:296:GLU:HB2   | 1.96                     | 0.48              |
| 7:K:379:ARG:O     | 7:K:383:GLU:N     | 2.41                     | 0.48              |
| 13:V:258:LYS:C    | 13:V:258:LYS:HZ2  | 2.22                     | 0.48              |
| 15:X:7:DG:C2'     | 15:X:8:DT:H5''    | 2.44                     | 0.48              |
| 15:X:48:DC:H2''   | 15:X:49:DT:C5     | 2.48                     | 0.48              |
| 1:A:32:HIS:HB2    | 1:A:49:PRO:CG     | 2.43                     | 0.47              |
| 5:I:754:PHE:CE1   | 5:I:755:LYS:HG3   | 2.48                     | 0.47              |
| 7:K:89:LEU:CD2    | 7:K:90:ASP:H      | 2.25                     | 0.47              |
| 7:K:131:SER:OG    | 7:K:147:ILE:HG23  | 2.14                     | 0.47              |
| 11:U:151:ILE:O    | 11:U:152:VAL:C    | 2.56                     | 0.47              |
| 11:U:363:ASP:O    | 13:V:95:TRP:CH2   | 2.66                     | 0.47              |
| 13:V:264:ARG:HH11 | 13:V:264:ARG:CG   | 2.17                     | 0.47              |
| 4:D:38:ALA:HB3    | 4:D:46:ILE:HD11   | 1.96                     | 0.47              |
| 3:G:73:GLU:HB2    | 4:H:25:ASN:OD1    | 2.14                     | 0.47              |
| 5:I:814:MET:SD    | 5:I:819:GLN:HA    | 2.54                     | 0.47              |
| 5:I:2037:LEU:HD11 | 5:I:2039:GLN:CD   | 2.39                     | 0.47              |
| 7:K:94:ILE:HA     | 7:K:122:VAL:O     | 2.13                     | 0.47              |
| 7:K:98:PRO:HD2    | 7:K:106:GLN:OE1   | 2.14                     | 0.47              |
| 7:K:377:VAL:HG23  | 7:K:393:LYS:HZ2   | 1.79                     | 0.47              |
| 9:M:196:ASN:OD1   | 9:M:197:SER:N     | 2.47                     | 0.47              |
| 9:M:425:ILE:CG2   | 9:M:430:VAL:HG23  | 2.43                     | 0.47              |
| 9:O:135:VAL:HG12  | 9:O:189:ASP:O     | 2.14                     | 0.47              |
| 12:T:340:ILE:HD13 | 13:V:172:VAL:CG1  | 2.44                     | 0.47              |
| 11:U:367:PRO:HD3  | 13:V:95:TRP:CG    | 2.49                     | 0.47              |
| 13:V:143:TYR:CD1  | 13:V:143:TYR:C    | 2.92                     | 0.47              |
| 13:V:265:SER:OG   | 14:W:198:LYS:HB2  | 2.14                     | 0.47              |
| 1:A:52:LEU:O      | 1:A:56:LEU:HG     | 2.14                     | 0.47              |
| 1:E:49:VAL:HG21   | 2:F:118:TYR:CE2   | 2.49                     | 0.47              |
| 5:I:129:GLU:CG    | 13:V:196:TYR:CE2  | 2.98                     | 0.47              |
| 5:I:888:MET:HE2   | 15:X:51:DG:N1     | 2.29                     | 0.47              |
| 5:I:2088:ARG:HG3  | 5:I:2115:ILE:HG22 | 1.97                     | 0.47              |
| 7:K:220:MET:CE    | 8:L:122:PHE:CD2   | 2.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:K:371:ASP:HA    | 7:K:374:ASP:CG    | 2.39                     | 0.47              |
| 9:Q:323:ILE:O     | 9:Q:323:ILE:HG22  | 2.14                     | 0.47              |
| 10:R:412:VAL:HG11 | 10:R:428:ARG:HG2  | 1.96                     | 0.47              |
| 15:X:125:DC:H2''  | 15:X:126:DC:C6    | 2.49                     | 0.47              |
| 1:A:63:ILE:HG23   | 1:A:64:LEU:N      | 2.29                     | 0.47              |
| 5:I:2055:LEU:HD22 | 5:I:2060:HIS:CE1  | 2.49                     | 0.47              |
| 7:K:381:ASP:HA    | 7:K:384:GLU:OE1   | 2.14                     | 0.47              |
| 8:L:6:THR:O       | 8:L:9:ARG:NH1     | 2.47                     | 0.47              |
| 9:M:91:VAL:CG1    | 9:M:297:GLY:HA2   | 2.44                     | 0.47              |
| 13:V:265:SER:HB2  | 14:W:198:LYS:HD3  | 1.95                     | 0.47              |
| 15:X:28:DG:C2'    | 15:X:29:DG:H8     | 2.28                     | 0.47              |
| 15:X:141:DC:C2'   | 15:X:142:DT:H5'   | 2.41                     | 0.47              |
| 2:F:75:SER:N      | 2:F:86:ILE:HD11   | 2.29                     | 0.47              |
| 3:G:68:GLN:O      | 3:G:72:ARG:HG3    | 2.15                     | 0.47              |
| 9:M:313:THR:CB    | 9:M:316:HIS:HE1   | 2.25                     | 0.47              |
| 10:R:301:VAL:HG21 | 10:R:326:MET:HE2  | 1.96                     | 0.47              |
| 15:X:6:DT:H2''    | 15:X:7:DG:OP2     | 2.13                     | 0.47              |
| 1:A:66:LEU:N      | 1:A:66:LEU:HD23   | 2.30                     | 0.47              |
| 7:K:161:CYS:SG    | 7:K:309:MET:HE1   | 2.54                     | 0.47              |
| 7:K:334:TYR:HB2   | 7:K:349:VAL:HB    | 1.96                     | 0.47              |
| 7:K:375:MET:O     | 7:K:376:VAL:CB    | 2.62                     | 0.47              |
| 10:R:389:VAL:HG21 | 10:R:423:VAL:HG23 | 1.97                     | 0.47              |
| 13:V:261:ARG:HD3  | 14:W:198:LYS:HZ2  | 1.78                     | 0.47              |
| 16:Y:-112:DT:H1'  | 16:Y:-111:DC:C5'  | 2.44                     | 0.47              |
| 16:Y:-102:DC:H2'' | 16:Y:-101:DT:C7   | 2.36                     | 0.47              |
| 1:A:32:HIS:O      | 1:A:32:HIS:HD2    | 1.97                     | 0.47              |
| 1:A:72:ARG:CZ     | 8:L:154:VAL:HG11  | 2.43                     | 0.47              |
| 3:C:42:ARG:NE     | 16:Y:-78:DA:OP1   | 2.37                     | 0.47              |
| 1:E:68:ASN:CG     | 6:J:144:THR:HG21  | 2.40                     | 0.47              |
| 1:E:100:VAL:HG11  | 4:H:98:TYR:CD2    | 2.49                     | 0.47              |
| 3:G:107:THR:HG23  | 3:G:124:ILE:N     | 2.30                     | 0.47              |
| 5:I:921:ILE:HD12  | 5:I:1986:PRO:HB2  | 1.96                     | 0.47              |
| 5:I:1886:LEU:HD21 | 7:K:315:LYS:CE    | 2.41                     | 0.47              |
| 7:K:172:ARG:NH1   | 8:L:101:TYR:CE2   | 2.83                     | 0.47              |
| 7:K:189:SER:OG    | 7:K:195:VAL:N     | 2.47                     | 0.47              |
| 8:L:38:ASP:OD1    | 8:L:39:ASN:N      | 2.44                     | 0.47              |
| 10:P:348:ILE:H    | 10:P:348:ILE:HD13 | 1.78                     | 0.47              |
| 10:R:408:ALA:HB3  | 10:R:429:VAL:HG11 | 1.96                     | 0.47              |
| 12:T:186:TYR:HB2  | 13:V:173:VAL:HG21 | 1.97                     | 0.47              |
| 13:V:244:GLU:HG2  | 13:V:248:LEU:HG   | 1.96                     | 0.47              |
| 13:V:254:ILE:HG13 | 13:V:255:GLU:OE1  | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:V:261:ARG:CD   | 14:W:198:LYS:HZ2  | 2.28                     | 0.47              |
| 15:X:8:DT:C2'     | 15:X:9:DA:H5'     | 2.45                     | 0.47              |
| 15:X:11:DA:C2'    | 15:X:12:DT:H71    | 2.45                     | 0.47              |
| 16:Y:-8:DA:H2''   | 16:Y:-7:DC:C6     | 2.49                     | 0.47              |
| 2:B:102:GLU:O     | 2:B:103:LEU:C     | 2.58                     | 0.47              |
| 3:C:121:PRO:HA    | 4:D:50:ILE:HD11   | 1.96                     | 0.47              |
| 1:E:64:GLU:O      | 2:F:46:HIS:HE1    | 1.98                     | 0.47              |
| 5:I:116:GLU:OE2   | 13:V:240:GLN:HG3  | 2.15                     | 0.47              |
| 5:I:163:ARG:CA    | 5:I:166:VAL:HG22  | 2.44                     | 0.47              |
| 5:I:694:LYS:CB    | 5:I:719:HIS:CD2   | 2.92                     | 0.47              |
| 5:I:892:ASN:CG    | 15:X:51:DG:H4'    | 2.40                     | 0.47              |
| 7:K:11:TYR:HB2    | 7:K:152:TYR:CZ    | 2.49                     | 0.47              |
| 7:K:79:PHE:HB3    | 7:K:88:PHE:HE1    | 1.79                     | 0.47              |
| 7:K:200:HIS:O     | 7:K:204:GLN:HG3   | 2.14                     | 0.47              |
| 7:K:224:LYS:CB    | 8:L:122:PHE:CE2   | 2.94                     | 0.47              |
| 9:Q:395:GLY:O     | 9:Q:399:THR:HG23  | 2.14                     | 0.47              |
| 12:T:184:ASP:HB3  | 13:V:170:ARG:HH11 | 1.80                     | 0.47              |
| 15:X:87:DT:H2''   | 15:X:88:DT:H72    | 1.96                     | 0.47              |
| 1:A:63:ILE:HG12   | 1:A:88:ILE:HD11   | 1.97                     | 0.47              |
| 3:G:106:ASP:O     | 3:G:127:ALA:HB2   | 2.15                     | 0.47              |
| 5:I:742:TYR:CD1   | 5:I:769:ARG:HB2   | 2.50                     | 0.47              |
| 5:I:975:LEU:HD23  | 5:I:1901:LEU:HD13 | 1.96                     | 0.47              |
| 9:M:394:LEU:HD13  | 9:M:430:VAL:HG11  | 1.97                     | 0.47              |
| 10:N:110:SER:OG   | 10:N:113:MET:O    | 2.32                     | 0.47              |
| 9:O:401:THR:O     | 9:O:402:THR:CG2   | 2.63                     | 0.47              |
| 13:V:179:ASP:HB3  | 13:V:183:PHE:CD2  | 2.50                     | 0.47              |
| 15:X:141:DC:C6    | 15:X:141:DC:H5''  | 2.50                     | 0.47              |
| 5:I:2030:THR:HG21 | 9:O:199:ALA:CB    | 2.45                     | 0.47              |
| 5:I:2131:ASP:O    | 5:I:2132:THR:OG1  | 2.23                     | 0.47              |
| 13:V:270:LYS:HD3  | 13:V:270:LYS:HA   | 1.59                     | 0.47              |
| 1:A:66:LEU:CD1    | 1:A:91:ASP:HB2    | 2.45                     | 0.46              |
| 7:K:371:ASP:O     | 7:K:375:MET:HG2   | 2.15                     | 0.46              |
| 7:K:377:VAL:CG2   | 7:K:389:VAL:HG22  | 2.44                     | 0.46              |
| 9:M:135:VAL:HG22  | 9:M:161:LEU:HD21  | 1.96                     | 0.46              |
| 11:U:262:PHE:HA   | 11:U:273:GLY:HA3  | 1.96                     | 0.46              |
| 13:V:264:ARG:HH12 | 14:W:194:ILE:HG21 | 1.80                     | 0.46              |
| 15:X:68:DG:H1'    | 15:X:69:DG:N7     | 2.30                     | 0.46              |
| 1:A:95:ASN:O      | 1:A:99:GLY:N      | 2.49                     | 0.46              |
| 1:E:80:PRO:HA     | 1:E:83:LEU:HB2    | 1.96                     | 0.46              |
| 7:K:160:TYR:OH    | 7:K:165:LYS:HD3   | 2.15                     | 0.46              |
| 7:K:228:GLU:O     | 7:K:229:GLU:CG    | 2.63                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:K:299:VAL:HG11  | 7:K:340:LEU:HB3   | 1.96                     | 0.46              |
| 7:K:311:PRO:O     | 7:K:315:LYS:HD3   | 2.16                     | 0.46              |
| 15:X:112:DA:H2''  | 15:X:113:DC:H6    | 1.81                     | 0.46              |
| 1:A:80:ILE:HG13   | 1:A:82:ARG:H      | 1.81                     | 0.46              |
| 1:E:42:ARG:HA     | 15:X:112:DA:OP1   | 2.15                     | 0.46              |
| 3:G:95:ALA:CB     | 4:H:90:LEU:HD11   | 2.45                     | 0.46              |
| 5:I:167:ARG:HD2   | 15:X:31:DG:O3'    | 2.14                     | 0.46              |
| 5:I:843:VAL:HG13  | 5:I:844:ASP:N     | 2.31                     | 0.46              |
| 7:K:198:GLU:HB2   | 7:K:201:VAL:CG2   | 2.46                     | 0.46              |
| 7:K:332:ARG:O     | 7:K:336:GLU:CG    | 2.61                     | 0.46              |
| 13:V:268:LEU:HD12 | 14:W:194:ILE:HG21 | 1.97                     | 0.46              |
| 15:X:38:DG:H2''   | 15:X:39:DA:C8     | 2.51                     | 0.46              |
| 15:X:54:DG:H2'    | 15:X:54:DG:P      | 2.55                     | 0.46              |
| 16:Y:-79:DT:H2''  | 16:Y:-78:DA:OP2   | 2.15                     | 0.46              |
| 1:A:32:HIS:HB2    | 1:A:49:PRO:HB3    | 1.94                     | 0.46              |
| 3:C:49:ARG:HD3    | 15:X:6:DT:O3'     | 2.15                     | 0.46              |
| 5:I:654:ILE:HA    | 5:I:657:LEU:HD12  | 1.97                     | 0.46              |
| 5:I:1904:ILE:HD13 | 10:R:211:ARG:HG2  | 1.98                     | 0.46              |
| 10:P:394:GLY:HA3  | 10:P:402:ALA:HB2  | 1.96                     | 0.46              |
| 10:R:205:LEU:CG   | 10:R:225:VAL:HG22 | 2.43                     | 0.46              |
| 13:V:237:THR:OG1  | 13:V:238:PRO:HD3  | 2.15                     | 0.46              |
| 13:V:245:GLU:HA   | 13:V:248:LEU:HD12 | 1.97                     | 0.46              |
| 15:X:6:DT:H1'     | 15:X:7:DG:H5'     | 1.97                     | 0.46              |
| 16:Y:-81:DC:H2''  | 16:Y:-80:DG:O5'   | 2.15                     | 0.46              |
| 2:B:73:GLU:HB3    | 2:B:94:ALA:HB1    | 1.96                     | 0.46              |
| 3:G:107:THR:CB    | 3:G:124:ILE:HG12  | 2.46                     | 0.46              |
| 5:I:201:ASP:OD1   | 5:I:202:VAL:N     | 2.47                     | 0.46              |
| 5:I:918:THR:O     | 5:I:918:THR:HG23  | 2.16                     | 0.46              |
| 5:I:1930:GLN:HB3  | 5:I:1931:PRO:HD3  | 1.98                     | 0.46              |
| 7:K:78:LEU:O      | 7:K:83:MET:HB2    | 2.16                     | 0.46              |
| 7:K:128:GLY:CA    | 7:K:147:ILE:HG13  | 2.45                     | 0.46              |
| 7:K:164:LYS:NZ    | 7:K:166:LYS:HD3   | 2.31                     | 0.46              |
| 8:L:8:VAL:O       | 8:L:9:ARG:C       | 2.58                     | 0.46              |
| 13:V:182:GLN:C    | 13:V:183:PHE:HD1  | 2.22                     | 0.46              |
| 15:X:41:DT:H2''   | 15:X:42:DA:H5'    | 1.97                     | 0.46              |
| 15:X:120:DA:H8    | 15:X:120:DA:H5''  | 1.80                     | 0.46              |
| 3:C:110:CYS:O     | 3:C:113:HIS:HB3   | 2.16                     | 0.46              |
| 5:I:916:PHE:O     | 5:I:1983:VAL:HG13 | 2.16                     | 0.46              |
| 7:K:286:ASP:OD1   | 7:K:286:ASP:N     | 2.48                     | 0.46              |
| 7:K:319:LEU:CD1   | 7:K:330:ARG:HA    | 2.46                     | 0.46              |
| 10:P:349:ASP:OD1  | 10:P:353:ARG:NH1  | 2.49                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:V:145:LEU:HB3  | 13:V:146:TYR:CE1  | 2.51                     | 0.46              |
| 13:V:224:ARG:O    | 13:V:228:GLU:HG3  | 2.16                     | 0.46              |
| 1:A:27:PRO:HG3    | 1:A:30:ARG:HE     | 1.80                     | 0.46              |
| 4:D:23:ARG:NH2    | 14:W:81:VAL:HG13  | 2.31                     | 0.46              |
| 4:D:79:LYS:N      | 15:X:101:DA:OP2   | 2.36                     | 0.46              |
| 7:K:36:ARG:NE     | 7:K:36:ARG:CA     | 2.78                     | 0.46              |
| 7:K:51:PRO:HG2    | 7:K:241:PHE:CE1   | 2.51                     | 0.46              |
| 9:M:333:ARG:O     | 9:M:348:HIS:HA    | 2.15                     | 0.46              |
| 9:O:171:LYS:C     | 9:O:172:LEU:HD22  | 2.41                     | 0.46              |
| 11:U:162:THR:HG21 | 11:U:277:THR:HG22 | 1.96                     | 0.46              |
| 13:V:222:HIS:CE1  | 13:V:226:ARG:HB2  | 2.49                     | 0.46              |
| 13:V:239:GLU:HB2  | 13:V:240:GLN:NE2  | 2.29                     | 0.46              |
| 15:X:45:DC:H2''   | 15:X:46:DC:C5'    | 2.39                     | 0.46              |
| 2:B:96:ARG:HE     | 13:V:64:ASP:HB3   | 1.81                     | 0.46              |
| 5:I:705:ARG:HH22  | 15:X:58:DA:P      | 2.38                     | 0.46              |
| 7:K:62:LYS:CD     | 7:K:172:ARG:HH12  | 2.28                     | 0.46              |
| 9:M:317:ARG:HD2   | 10:R:104:ALA:HB2  | 1.98                     | 0.46              |
| 11:S:103:VAL:O    | 11:S:132:MET:HA   | 2.16                     | 0.46              |
| 13:V:261:ARG:HD3  | 14:W:198:LYS:NZ   | 2.31                     | 0.46              |
| 13:V:272:ILE:HD13 | 14:W:191:SER:CB   | 2.46                     | 0.46              |
| 1:E:20:ARG:HD2    | 2:F:118:TYR:CD1   | 2.50                     | 0.46              |
| 5:I:977:VAL:O     | 5:I:977:VAL:HG12  | 2.16                     | 0.46              |
| 7:K:114:PHE:O     | 7:K:118:GLN:N     | 2.49                     | 0.46              |
| 7:K:135:TYR:CE2   | 7:K:145:CYS:HB3   | 2.50                     | 0.46              |
| 12:T:338:ILE:HD13 | 13:V:230:LEU:HD22 | 1.96                     | 0.46              |
| 13:V:247:LEU:HA   | 13:V:250:GLU:HB2  | 1.98                     | 0.46              |
| 13:V:261:ARG:HA   | 14:W:198:LYS:HE3  | 1.97                     | 0.46              |
| 16:Y:-139:DA:H2'  | 16:Y:-138:DT:H72  | 1.97                     | 0.46              |
| 1:A:58:TYR:HB2    | 2:B:110:GLU:CD    | 2.41                     | 0.46              |
| 10:R:211:ARG:HG2  | 10:R:212:ALA:H    | 1.81                     | 0.46              |
| 11:U:165:ILE:HG22 | 11:U:170:ALA:HA   | 1.97                     | 0.46              |
| 11:U:188:TYR:CZ   | 11:U:192:ILE:HD11 | 2.51                     | 0.46              |
| 13:V:259:LYS:C    | 13:V:261:ARG:N    | 2.73                     | 0.46              |
| 16:Y:-111:DC:H2'  | 16:Y:-111:DC:O5'  | 2.16                     | 0.46              |
| 1:A:114:ALA:HA    | 1:A:117:LEU:HD12  | 1.97                     | 0.45              |
| 7:K:160:TYR:CZ    | 7:K:165:LYS:HB2   | 2.51                     | 0.45              |
| 7:K:200:HIS:CE1   | 7:K:201:VAL:HG22  | 2.51                     | 0.45              |
| 7:K:310:GLN:HA    | 7:K:313:PHE:HB2   | 1.98                     | 0.45              |
| 13:V:59:ALA:O     | 13:V:63:SER:HB2   | 2.15                     | 0.45              |
| 13:V:259:LYS:NZ   | 13:V:259:LYS:H    | 2.14                     | 0.45              |
| 1:A:32:HIS:HB2    | 1:A:49:PRO:HG3    | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:I:2088:ARG:HG3  | 5:I:2115:ILE:C    | 2.41                     | 0.45              |
| 7:K:6:LEU:HB2     | 7:K:94:ILE:O      | 2.16                     | 0.45              |
| 7:K:93:ILE:HG23   | 7:K:122:VAL:HG23  | 1.98                     | 0.45              |
| 7:K:315:LYS:HE3   | 7:K:315:LYS:HB2   | 1.55                     | 0.45              |
| 10:N:117:GLU:HA   | 10:N:120:THR:HG22 | 1.98                     | 0.45              |
| 13:V:261:ARG:HA   | 14:W:198:LYS:NZ   | 2.31                     | 0.45              |
| 15:X:109:DA:H2''  | 15:X:110:DC:OP2   | 2.17                     | 0.45              |
| 3:C:103:LEU:HD22  | 4:D:57:VAL:HG11   | 1.97                     | 0.45              |
| 2:F:75:SER:CA     | 2:F:86:ILE:HD11   | 2.46                     | 0.45              |
| 7:K:181:THR:OG1   | 7:K:206:LYS:NZ    | 2.48                     | 0.45              |
| 9:M:40:VAL:CG2    | 9:M:377:ILE:CD1   | 2.94                     | 0.45              |
| 10:P:180:GLU:O    | 10:P:184:LYS:HG2  | 2.17                     | 0.45              |
| 13:V:257:ARG:H    | 13:V:257:ARG:HG2  | 1.47                     | 0.45              |
| 2:B:100:PRO:HG2   | 2:B:103:LEU:HB2   | 1.98                     | 0.45              |
| 3:C:104:PHE:HZ    | 4:D:54:THR:HG1    | 1.63                     | 0.45              |
| 1:E:66:ALA:CB     | 1:E:83:LEU:HD23   | 2.47                     | 0.45              |
| 2:F:65:ASP:OD2    | 4:H:98:TYR:OH     | 2.31                     | 0.45              |
| 7:K:11:TYR:HB2    | 7:K:152:TYR:CG    | 2.51                     | 0.45              |
| 7:K:156:HIS:HB3   | 7:K:170:ILE:HD11  | 1.99                     | 0.45              |
| 7:K:378:THR:HB    | 7:K:380:GLU:CD    | 2.41                     | 0.45              |
| 13:V:91:LYS:NZ    | 13:V:91:LYS:HB3   | 2.22                     | 0.45              |
| 13:V:98:MET:HB3   | 13:V:120:GLU:OE1  | 2.16                     | 0.45              |
| 15:X:5:DA:H2'     | 15:X:6:DT:C7      | 2.47                     | 0.45              |
| 15:X:23:DT:C2'    | 15:X:24:DG:C8     | 3.00                     | 0.45              |
| 1:A:48:ALA:N      | 1:A:49:PRO:HD2    | 2.32                     | 0.45              |
| 2:B:28:ARG:HA     | 2:B:28:ARG:HE     | 1.79                     | 0.45              |
| 1:E:28:GLY:HA3    | 16:Y:-117:DA:H3'  | 1.96                     | 0.45              |
| 1:E:51:LEU:O      | 1:E:55:LEU:HG     | 2.16                     | 0.45              |
| 3:G:59:GLU:H      | 4:H:40:ARG:HH22   | 1.65                     | 0.45              |
| 7:K:230:ASN:O     | 7:K:232:VAL:N     | 2.50                     | 0.45              |
| 9:O:366:TYR:OH    | 17:O:501:ADP:N7   | 2.41                     | 0.45              |
| 7:K:75:TRP:CZ3    | 7:K:113:LEU:HD23  | 2.52                     | 0.45              |
| 7:K:230:ASN:C     | 7:K:231:THR:HG1   | 2.21                     | 0.45              |
| 13:V:183:PHE:CD1  | 13:V:183:PHE:N    | 2.83                     | 0.45              |
| 15:X:59:DA:H1'    | 15:X:60:DA:H5''   | 1.97                     | 0.45              |
| 16:Y:-13:DT:C4    | 16:Y:-12:DA:N6    | 2.85                     | 0.45              |
| 1:E:62:ILE:HG12   | 1:E:93:LEU:HD13   | 1.97                     | 0.45              |
| 1:E:111:ILE:CG2   | 1:E:116:LEU:HG    | 2.47                     | 0.45              |
| 3:G:129:ARG:HA    | 3:G:134:ARG:HB2   | 1.98                     | 0.45              |
| 5:I:733:GLN:OE1   | 5:I:736:ARG:NH2   | 2.50                     | 0.45              |
| 5:I:2072:LEU:HD22 | 5:I:2115:ILE:HG22 | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:O:264:MET:HE3   | 9:O:268:LYS:HE3   | 1.99                     | 0.45              |
| 9:Q:268:LYS:O     | 9:Q:268:LYS:HG2   | 2.17                     | 0.45              |
| 13:V:220:ALA:CB   | 13:V:224:ARG:NH2  | 2.79                     | 0.45              |
| 15:X:99:DA:C1'    | 15:X:100:DG:H5'   | 2.41                     | 0.45              |
| 16:Y:-1:DG:C2'    | 16:Y:0:DT:H5''    | 2.47                     | 0.45              |
| 1:A:18:ARG:HH22   | 1:A:36:ARG:NH1    | 2.15                     | 0.45              |
| 1:E:18:SER:HB3    | 1:E:27:VAL:H      | 1.82                     | 0.45              |
| 1:E:84:GLN:O      | 1:E:88:ARG:HG2    | 2.17                     | 0.45              |
| 1:E:88:ARG:NH2    | 1:E:100:VAL:O     | 2.49                     | 0.45              |
| 5:I:2087:LEU:HD11 | 5:I:2104:ARG:HH11 | 1.71                     | 0.45              |
| 7:K:7:ASP:O       | 7:K:9:GLY:N       | 2.47                     | 0.45              |
| 7:K:171:ILE:HG21  | 7:K:292:MET:HE1   | 1.99                     | 0.45              |
| 7:K:379:ARG:CZ    | 7:K:379:ARG:HB3   | 2.47                     | 0.45              |
| 9:O:276:ARG:HH11  | 9:O:276:ARG:CG    | 2.30                     | 0.45              |
| 9:Q:233:GLU:HG3   | 9:Q:233:GLU:O     | 2.17                     | 0.45              |
| 13:V:211:THR:O    | 13:V:212:ASP:C    | 2.60                     | 0.45              |
| 15:X:49:DT:C6     | 15:X:50:DT:H71    | 2.52                     | 0.45              |
| 16:Y:-10:DA:H2''  | 16:Y:-9:DT:H5'    | 1.99                     | 0.45              |
| 1:A:82:ARG:HA     | 1:A:106:GLY:O     | 2.16                     | 0.45              |
| 1:A:94:LEU:HD23   | 2:B:103:LEU:HD21  | 1.99                     | 0.45              |
| 2:B:88:SER:HA     | 2:B:91:ILE:HB     | 1.98                     | 0.45              |
| 3:C:82:LEU:HD23   | 3:C:82:LEU:HA     | 1.80                     | 0.45              |
| 3:G:103:LEU:CD1   | 3:G:128:ARG:HG2   | 2.47                     | 0.45              |
| 5:I:754:PHE:CZ    | 5:I:801:ARG:HD3   | 2.52                     | 0.45              |
| 7:K:214:GLN:NE2   | 7:K:332:ARG:HG2   | 2.32                     | 0.45              |
| 7:K:344:ASP:OD1   | 7:K:344:ASP:N     | 2.50                     | 0.45              |
| 8:L:87:LEU:C      | 8:L:87:LEU:HD13   | 2.42                     | 0.45              |
| 9:M:192:TYR:O     | 9:M:192:TYR:CG    | 2.70                     | 0.45              |
| 9:O:308:ASP:OD1   | 9:O:309:ILE:N     | 2.50                     | 0.45              |
| 10:R:416:ARG:O    | 10:R:416:ARG:HG2  | 2.17                     | 0.45              |
| 13:V:147:LEU:CD2  | 13:V:201:LYS:HB3  | 2.47                     | 0.45              |
| 1:A:32:HIS:HB3    | 1:A:36:ARG:HH12   | 1.82                     | 0.45              |
| 1:A:117:LEU:HB3   | 1:A:118:PRO:CD    | 2.47                     | 0.45              |
| 2:F:34:TYR:CE2    | 2:F:63:VAL:HB     | 2.52                     | 0.45              |
| 7:K:82:GLU:N      | 7:K:82:GLU:OE1    | 2.49                     | 0.45              |
| 7:K:308:GLU:O     | 7:K:311:PRO:HD2   | 2.17                     | 0.45              |
| 7:K:334:TYR:O     | 7:K:335:SER:C     | 2.59                     | 0.45              |
| 9:O:428:GLU:OE1   | 9:O:429:HIS:ND1   | 2.50                     | 0.45              |
| 13:V:94:PRO:HD2   | 13:V:117:ALA:CB   | 2.47                     | 0.45              |
| 13:V:255:GLU:CA   | 13:V:259:LYS:HE2  | 2.47                     | 0.45              |
| 16:Y:-53:DG:C5    | 16:Y:-52:DC:C4    | 3.05                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:102:GLU:OE1  | 2:B:102:GLU:HA    | 2.18                     | 0.44              |
| 4:H:84:MET:HE3   | 4:H:88:TYR:CE1    | 2.52                     | 0.44              |
| 9:M:40:VAL:HG21  | 9:M:377:ILE:CD1   | 2.46                     | 0.44              |
| 13:V:161:PHE:CE1 | 13:V:198:ILE:HG21 | 2.52                     | 0.44              |
| 15:X:44:DT:H2"   | 15:X:45:DC:C6     | 2.51                     | 0.44              |
| 1:A:26:PHE:HE2   | 2:B:63:VAL:CG2    | 2.30                     | 0.44              |
| 1:A:81:PRO:HB3   | 1:A:104:ALA:O     | 2.17                     | 0.44              |
| 3:C:61:LEU:H     | 3:C:97:GLU:CD     | 2.24                     | 0.44              |
| 7:K:35:ALA:O     | 7:K:36:ARG:C      | 2.60                     | 0.44              |
| 7:K:112:ILE:HG23 | 7:K:116:GLU:OE1   | 2.16                     | 0.44              |
| 7:K:307:GLU:O    | 7:K:310:GLN:HG3   | 2.17                     | 0.44              |
| 9:M:135:VAL:HG22 | 9:M:161:LEU:HD23  | 1.97                     | 0.44              |
| 9:M:357:ARG:HB3  | 10:R:400:ARG:HD2  | 1.99                     | 0.44              |
| 10:P:33:LEU:HD23 | 10:P:39:PRO:HA    | 1.97                     | 0.44              |
| 11:U:193:LEU:C   | 11:U:195:GLU:H    | 2.22                     | 0.44              |
| 15:X:93:DG:C4    | 15:X:94:DG:C8     | 3.06                     | 0.44              |
| 1:A:33:ARG:NH2   | 2:B:32:GLU:OE1    | 2.41                     | 0.44              |
| 1:A:39:ASN:HD22  | 1:E:40:ALA:HA     | 1.82                     | 0.44              |
| 1:A:59:LEU:HG    | 1:A:59:LEU:H      | 1.54                     | 0.44              |
| 1:A:59:LEU:HD13  | 2:B:66:ILE:HG13   | 1.99                     | 0.44              |
| 1:E:32:ARG:O     | 1:E:36:LYS:HB2    | 2.17                     | 0.44              |
| 3:G:129:ARG:HD3  | 3:G:134:ARG:HH21  | 1.82                     | 0.44              |
| 7:K:21:ASN:O     | 7:K:22:VAL:C      | 2.60                     | 0.44              |
| 7:K:295:PRO:HG2  | 7:K:296:GLU:OE1   | 2.17                     | 0.44              |
| 7:K:334:TYR:O    | 7:K:337:VAL:HG22  | 2.17                     | 0.44              |
| 7:K:335:SER:HA   | 7:K:338:ARG:NH2   | 2.32                     | 0.44              |
| 9:O:50:GLY:O     | 9:O:53:VAL:HG22   | 2.17                     | 0.44              |
| 9:Q:49:CYS:HB2   | 9:Q:83:ILE:HD11   | 1.98                     | 0.44              |
| 11:U:124:PHE:HB3 | 13:V:91:LYS:HE2   | 1.98                     | 0.44              |
| 15:X:52:DG:C4    | 15:X:53:DC:C5     | 3.04                     | 0.44              |
| 1:A:32:HIS:CB    | 1:A:49:PRO:HB3    | 2.48                     | 0.44              |
| 3:C:82:LEU:HD11  | 4:D:70:VAL:HG22   | 1.99                     | 0.44              |
| 3:C:103:LEU:HA   | 3:C:131:ARG:NH2   | 2.33                     | 0.44              |
| 1:E:29:ARG:NH1   | 2:F:33:SER:O      | 2.44                     | 0.44              |
| 5:I:612:LEU:O    | 5:I:614:LEU:N     | 2.50                     | 0.44              |
| 7:K:189:SER:CB   | 7:K:194:HIS:HA    | 2.47                     | 0.44              |
| 7:K:213:SER:HB3  | 7:K:275:PHE:HB2   | 1.98                     | 0.44              |
| 7:K:279:GLU:HG2  | 7:K:283:ASN:OD1   | 2.18                     | 0.44              |
| 10:N:298:ILE:O   | 10:N:301:VAL:HG23 | 2.17                     | 0.44              |
| 10:N:298:ILE:CG2 | 10:N:301:VAL:HG22 | 2.48                     | 0.44              |
| 13:V:56:GLU:OE1  | 13:V:56:GLU:N     | 2.50                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:V:152:TRP:CE2  | 13:V:194:ARG:HD3  | 2.52                     | 0.44              |
| 13:V:214:LYS:N    | 13:V:214:LYS:HD2  | 2.33                     | 0.44              |
| 13:V:264:ARG:CB   | 14:W:198:LYS:HE3  | 2.47                     | 0.44              |
| 1:A:59:LEU:CD1    | 2:B:66:ILE:HG13   | 2.48                     | 0.44              |
| 1:E:106:GLY:CA    | 3:G:58:THR:HG22   | 2.38                     | 0.44              |
| 2:F:29:SER:O      | 2:F:31:LYS:N      | 2.50                     | 0.44              |
| 3:G:57:SER:O      | 4:H:40:ARG:NH2    | 2.51                     | 0.44              |
| 3:G:63:ARG:HE     | 15:X:59:DA:H4'    | 1.81                     | 0.44              |
| 5:I:752:LYS:HE2   | 16:Y:-52:DC:OP2   | 2.18                     | 0.44              |
| 5:I:2067:GLN:O    | 5:I:2068:MET:HB2  | 2.18                     | 0.44              |
| 7:K:99:TYR:HE2    | 7:K:158:VAL:CG2   | 2.31                     | 0.44              |
| 7:K:159:PRO:HB2   | 7:K:166:LYS:HE3   | 2.00                     | 0.44              |
| 7:K:224:LYS:HZ2   | 7:K:224:LYS:HG3   | 1.50                     | 0.44              |
| 7:K:287:ILE:HD13  | 7:K:287:ILE:HA    | 1.80                     | 0.44              |
| 10:N:301:VAL:HG21 | 10:N:326:MET:HB3  | 1.97                     | 0.44              |
| 13:V:264:ARG:HG2  | 13:V:264:ARG:NH1  | 2.17                     | 0.44              |
| 15:X:127:DT:H6    | 15:X:127:DT:H2'   | 1.65                     | 0.44              |
| 1:A:79:ILE:HA     | 1:A:83:HIS:ND1    | 2.32                     | 0.44              |
| 3:C:130:ILE:CG2   | 3:G:130:ILE:HB    | 2.48                     | 0.44              |
| 5:I:664:LYS:HA    | 5:I:664:LYS:HE2   | 1.99                     | 0.44              |
| 5:I:921:ILE:O     | 5:I:921:ILE:HG13  | 2.17                     | 0.44              |
| 5:I:2050:VAL:O    | 5:I:2054:GLN:HG2  | 2.18                     | 0.44              |
| 7:K:102:PHE:O     | 7:K:103:THR:C     | 2.60                     | 0.44              |
| 7:K:184:LEU:O     | 7:K:185:LYS:C     | 2.61                     | 0.44              |
| 7:K:229:GLU:CG    | 7:K:230:ASN:H     | 2.30                     | 0.44              |
| 7:K:282:PHE:HB3   | 7:K:332:ARG:NH2   | 2.32                     | 0.44              |
| 7:K:352:PRO:O     | 7:K:355:PRO:HD3   | 2.17                     | 0.44              |
| 12:T:374:PRO:HD2  | 13:V:241:VAL:HG21 | 1.99                     | 0.44              |
| 13:V:262:GLU:O    | 13:V:266:GLN:HG2  | 2.17                     | 0.44              |
| 15:X:92:DC:H2''   | 15:X:93:DG:C5'    | 2.48                     | 0.44              |
| 2:B:41:VAL:O      | 2:B:45:VAL:HG13   | 2.18                     | 0.44              |
| 3:C:60:LEU:CD1    | 3:C:90:MET:HE1    | 2.48                     | 0.44              |
| 5:I:128:PRO:HG3   | 13:V:218:PHE:HA   | 1.99                     | 0.44              |
| 5:I:612:LEU:HD22  | 5:I:612:LEU:N     | 2.33                     | 0.44              |
| 5:I:927:SER:C     | 5:I:1993:CYS:SG   | 3.01                     | 0.44              |
| 5:I:948:LEU:N     | 9:M:247:ASN:OD1   | 2.50                     | 0.44              |
| 7:K:150:SER:O     | 7:K:323:ASN:N     | 2.47                     | 0.44              |
| 7:K:302:ILE:HG23  | 7:K:313:PHE:CB    | 2.48                     | 0.44              |
| 7:K:336:GLU:HG2   | 7:K:336:GLU:H     | 1.48                     | 0.44              |
| 9:O:264:MET:HG2   | 9:O:266:PRO:HD3   | 2.00                     | 0.44              |
| 9:O:276:ARG:HH11  | 9:O:276:ARG:HG3   | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:R:49:GLN:NE2   | 10:R:360:THR:O    | 2.44                     | 0.44              |
| 15:X:55:DG:C2'    | 15:X:56:DT:H5''   | 2.45                     | 0.44              |
| 16:Y:-21:DG:H2'   | 16:Y:-20:DT:H6    | 1.82                     | 0.44              |
| 5:I:206:TRP:O     | 5:I:210:GLU:HG2   | 2.18                     | 0.44              |
| 5:I:2029:ARG:C    | 5:I:2030:THR:HG23 | 2.43                     | 0.44              |
| 7:K:44:GLN:HG3    | 7:K:77:TYR:HE2    | 1.81                     | 0.44              |
| 9:O:341:THR:O     | 9:O:342:GLU:CG    | 2.66                     | 0.44              |
| 12:T:337:ASP:HB3  | 13:V:227:LYS:HZ1  | 1.82                     | 0.44              |
| 13:V:264:ARG:NH2  | 14:W:198:LYS:HZ3  | 2.15                     | 0.44              |
| 16:Y:-75:DC:H2''  | 16:Y:-74:DG:O5'   | 2.18                     | 0.44              |
| 1:A:58:TYR:HH     | 2:B:106:HIS:HD1   | 1.55                     | 0.44              |
| 1:A:60:THR:HG21   | 2:B:63:VAL:HG22   | 1.98                     | 0.44              |
| 7:K:147:ILE:HG12  | 7:K:160:TYR:CE2   | 2.52                     | 0.44              |
| 7:K:265:GLU:HB2   | 7:K:267:ILE:CG2   | 2.47                     | 0.44              |
| 8:L:92:ASN:C      | 8:L:92:ASN:OD1    | 2.60                     | 0.44              |
| 10:R:74:LEU:HB2   | 10:R:354:LEU:HD13 | 2.00                     | 0.44              |
| 10:R:204:LYS:C    | 10:R:205:LEU:HD22 | 2.42                     | 0.44              |
| 10:R:430:TYR:O    | 10:R:438:ARG:NH2  | 2.51                     | 0.44              |
| 13:V:147:LEU:HD22 | 13:V:201:LYS:HB3  | 1.99                     | 0.44              |
| 13:V:238:PRO:HG2  | 13:V:239:GLU:HG3  | 1.99                     | 0.44              |
| 14:W:190:THR:HG22 | 14:W:194:ILE:CD1  | 2.47                     | 0.44              |
| 15:X:70:DA:H2''   | 15:X:71:DC:H5''   | 2.00                     | 0.44              |
| 16:Y:-21:DG:C2'   | 16:Y:-20:DT:C6    | 2.99                     | 0.44              |
| 1:A:25:GLN:O      | 2:B:37:TYR:CD1    | 2.71                     | 0.43              |
| 1:A:93:GLU:OE1    | 2:B:102:GLU:HB2   | 2.18                     | 0.43              |
| 2:B:73:GLU:OE2    | 2:B:97:LEU:HD13   | 2.17                     | 0.43              |
| 2:B:77:LEU:HD13   | 4:H:72:TYR:HE1    | 1.81                     | 0.43              |
| 2:F:99:LEU:HD12   | 2:F:107:ALA:HB3   | 2.00                     | 0.43              |
| 4:H:35:ARG:O      | 4:H:39:ARG:HG2    | 2.18                     | 0.43              |
| 7:K:236:TYR:H     | 7:K:269:ARG:HB2   | 1.82                     | 0.43              |
| 7:K:240:ASP:C     | 7:K:242:SER:H     | 2.26                     | 0.43              |
| 7:K:370:ASP:C     | 7:K:371:ASP:CG    | 2.87                     | 0.43              |
| 8:L:33:GLU:O      | 8:L:37:ASN:N      | 2.51                     | 0.43              |
| 10:P:324:LEU:HD12 | 10:P:324:LEU:O    | 2.18                     | 0.43              |
| 11:U:96:VAL:HG22  | 11:U:96:VAL:O     | 2.18                     | 0.43              |
| 11:U:121:GLN:OE1  | 13:V:114:TRP:HH2  | 2.01                     | 0.43              |
| 13:V:90:LYS:HB3   | 13:V:90:LYS:HE3   | 1.38                     | 0.43              |
| 13:V:187:SER:O    | 13:V:191:LEU:HG   | 2.18                     | 0.43              |
| 15:X:29:DG:H2''   | 15:X:30:DA:H8     | 1.83                     | 0.43              |
| 1:A:60:THR:HA     | 2:B:59:MET:CE     | 2.48                     | 0.43              |
| 1:A:96:LYS:HD2    | 1:A:96:LYS:C      | 2.41                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:92:GLN:HG3    | 2:B:108:VAL:HG13  | 1.99                     | 0.43              |
| 5:I:1886:LEU:HD11 | 7:K:312:HIS:CD2   | 2.53                     | 0.43              |
| 7:K:43:ASN:OD1    | 7:K:43:ASN:N      | 2.51                     | 0.43              |
| 7:K:81:LYS:HE3    | 7:K:81:LYS:HB3    | 1.58                     | 0.43              |
| 7:K:148:VAL:HB    | 7:K:319:LEU:HA    | 1.99                     | 0.43              |
| 7:K:269:ARG:HA    | 7:K:269:ARG:HD2   | 1.76                     | 0.43              |
| 9:M:275:LEU:HD13  | 10:R:260:LEU:HD23 | 1.99                     | 0.43              |
| 7:K:109:MET:O     | 7:K:110:ASN:C     | 2.59                     | 0.43              |
| 7:K:164:LYS:HD2   | 7:K:164:LYS:HA    | 1.57                     | 0.43              |
| 7:K:164:LYS:HZ2   | 7:K:164:LYS:HG3   | 1.69                     | 0.43              |
| 7:K:179:LEU:O     | 7:K:180:LEU:C     | 2.61                     | 0.43              |
| 7:K:205:VAL:HG11  | 7:K:269:ARG:NH2   | 2.33                     | 0.43              |
| 7:K:205:VAL:HA    | 7:K:208:ASP:HB2   | 2.00                     | 0.43              |
| 7:K:216:PHE:HE2   | 8:L:116:PHE:CZ    | 2.37                     | 0.43              |
| 7:K:375:MET:N     | 7:K:375:MET:SD    | 2.91                     | 0.43              |
| 7:K:376:VAL:HG22  | 7:K:377:VAL:H     | 1.84                     | 0.43              |
| 10:P:329:ASN:ND2  | 9:Q:353:ASP:OD2   | 2.47                     | 0.43              |
| 12:T:408:GLN:HA   | 13:V:105:ARG:HD2  | 2.01                     | 0.43              |
| 13:V:271:LEU:HB3  | 14:W:187:LYS:NZ   | 2.34                     | 0.43              |
| 15:X:99:DA:C2'    | 15:X:100:DG:H5'   | 2.49                     | 0.43              |
| 1:A:47:GLY:C      | 2:B:88:SER:HB2    | 2.43                     | 0.43              |
| 1:E:54:VAL:HG21   | 2:F:95:VAL:HG21   | 1.99                     | 0.43              |
| 1:E:62:ILE:HD12   | 2:F:62:PHE:CE2    | 2.53                     | 0.43              |
| 3:G:118:THR:HA    | 4:H:45:ARG:HB3    | 2.00                     | 0.43              |
| 5:I:938:LEU:C     | 9:M:234:ILE:HD11  | 2.43                     | 0.43              |
| 7:K:133:HIS:CE1   | 7:K:366:ILE:HG12  | 2.53                     | 0.43              |
| 7:K:157:ILE:HG12  | 7:K:173:ILE:HD11  | 2.01                     | 0.43              |
| 7:K:162:ARG:O     | 7:K:163:SER:OG    | 2.31                     | 0.43              |
| 7:K:330:ARG:C     | 7:K:330:ARG:HE    | 2.26                     | 0.43              |
| 15:X:7:DG:C2      | 16:Y:-6:DA:C2     | 3.06                     | 0.43              |
| 5:I:124:LEU:H     | 13:V:226:ARG:HH11 | 1.67                     | 0.43              |
| 7:K:3:THR:HB      | 7:K:94:ILE:HG22   | 2.01                     | 0.43              |
| 7:K:120:GLN:N     | 7:K:378:THR:HG21  | 2.34                     | 0.43              |
| 7:K:233:MET:CG    | 7:K:252:ARG:HG3   | 2.47                     | 0.43              |
| 9:M:384:ILE:HG22  | 9:M:386:ILE:HG23  | 2.01                     | 0.43              |
| 9:M:394:LEU:HD13  | 9:M:430:VAL:CG1   | 2.48                     | 0.43              |
| 13:V:203:ALA:HA   | 13:V:206:ARG:HD2  | 2.00                     | 0.43              |
| 15:X:5:DA:H2'     | 15:X:6:DT:H72     | 2.00                     | 0.43              |
| 15:X:126:DC:H5'   | 15:X:126:DC:C6    | 2.53                     | 0.43              |
| 16:Y:-144:DG:H2'' | 16:Y:-143:DG:H5'  | 2.00                     | 0.43              |
| 3:C:126:LEU:HD22  | 3:G:113:HIS:CD2   | 2.54                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:74:LYS:HD3    | 6:J:151:ARG:HD2   | 2.00                     | 0.43              |
| 2:F:65:ASP:OD2    | 2:F:69:ARG:NH2    | 2.38                     | 0.43              |
| 3:G:72:ARG:HH12   | 3:G:84:PHE:HB2    | 1.84                     | 0.43              |
| 7:K:75:TRP:HA     | 7:K:78:LEU:HD12   | 2.00                     | 0.43              |
| 7:K:148:VAL:HG22  | 7:K:157:ILE:HD12  | 2.00                     | 0.43              |
| 7:K:190:TYR:HB2   | 8:L:148:ARG:NH2   | 2.31                     | 0.43              |
| 13:V:96:LYS:HE2   | 13:V:120:GLU:OE1  | 2.19                     | 0.43              |
| 13:V:222:HIS:ND1  | 13:V:222:HIS:C    | 2.70                     | 0.43              |
| 16:Y:-30:DT:H2'   | 16:Y:-29:DC:C6    | 2.54                     | 0.43              |
| 1:A:85:GLN:NE2    | 1:A:89:ARG:HE     | 2.17                     | 0.43              |
| 1:A:89:ARG:CB     | 1:A:109:LEU:HD11  | 2.46                     | 0.43              |
| 3:G:63:ARG:HH21   | 15:X:59:DA:H5''   | 1.84                     | 0.43              |
| 5:I:128:PRO:CD    | 13:V:218:PHE:HA   | 2.48                     | 0.43              |
| 5:I:898:ARG:HA    | 5:I:898:ARG:NE    | 2.33                     | 0.43              |
| 5:I:930:LEU:C     | 5:I:930:LEU:HD23  | 2.43                     | 0.43              |
| 7:K:14:LYS:HA     | 7:K:23:SER:O      | 2.18                     | 0.43              |
| 7:K:156:HIS:HB3   | 7:K:170:ILE:CD1   | 2.49                     | 0.43              |
| 7:K:270:LEU:O     | 7:K:271:ALA:HB3   | 2.19                     | 0.43              |
| 7:K:317:ILE:HD12  | 7:K:349:VAL:HG22  | 2.00                     | 0.43              |
| 12:T:340:ILE:HG21 | 13:V:172:VAL:HG11 | 2.01                     | 0.43              |
| 13:V:244:GLU:O    | 13:V:245:GLU:C    | 2.62                     | 0.43              |
| 13:V:247:LEU:CD1  | 13:V:248:LEU:HD23 | 2.48                     | 0.43              |
| 15:X:138:DA:H2''  | 15:X:139:DT:C5    | 2.53                     | 0.43              |
| 1:A:26:PHE:CE2    | 2:B:63:VAL:HG11   | 2.53                     | 0.43              |
| 1:A:78:ARG:CZ     | 15:X:18:DA:H4'    | 2.49                     | 0.43              |
| 3:C:41:TYR:HB2    | 15:X:83:DG:OP1    | 2.18                     | 0.43              |
| 1:E:58:LEU:HD12   | 2:F:66:ILE:HG21   | 2.00                     | 0.43              |
| 3:G:116:ARG:NH2   | 3:G:122:LYS:HE3   | 2.34                     | 0.43              |
| 5:I:129:GLU:CG    | 13:V:196:TYR:HE2  | 2.32                     | 0.43              |
| 5:I:921:ILE:CG2   | 5:I:1986:PRO:CD   | 2.51                     | 0.43              |
| 7:K:103:THR:O     | 7:K:107:GLU:HB3   | 2.18                     | 0.43              |
| 7:K:128:GLY:C     | 7:K:147:ILE:HG13  | 2.43                     | 0.43              |
| 7:K:172:ARG:O     | 7:K:173:ILE:C     | 2.62                     | 0.43              |
| 7:K:184:LEU:HD12  | 7:K:184:LEU:HA    | 1.87                     | 0.43              |
| 7:K:302:ILE:HG23  | 7:K:313:PHE:HB3   | 2.01                     | 0.43              |
| 7:K:319:LEU:CD2   | 7:K:333:VAL:HG11  | 2.45                     | 0.43              |
| 7:K:366:ILE:HD13  | 7:K:366:ILE:HA    | 1.82                     | 0.43              |
| 9:M:40:VAL:HG21   | 9:M:377:ILE:HD11  | 2.00                     | 0.43              |
| 13:V:65:LYS:O     | 13:V:65:LYS:HG2   | 2.17                     | 0.43              |
| 13:V:136:PRO:HG3  | 13:V:199:CYS:SG   | 2.59                     | 0.43              |
| 13:V:147:LEU:HD11 | 13:V:198:ILE:HA   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 13:V:262:GLU:CG   | 14:W:202:LYS:CE  | 2.96                     | 0.43              |
| 1:A:26:PHE:CE2    | 2:B:63:VAL:HG21  | 2.54                     | 0.43              |
| 1:A:30:ARG:NH2    | 2:B:34:TYR:HA    | 2.31                     | 0.43              |
| 1:A:56:LEU:CD2    | 2:B:67:PHE:N     | 2.77                     | 0.43              |
| 5:I:2034:ASP:O    | 5:I:2035:LEU:HB2 | 2.19                     | 0.43              |
| 7:K:109:MET:SD    | 7:K:124:ARG:NH2  | 2.91                     | 0.43              |
| 7:K:118:GLN:C     | 7:K:379:ARG:HH12 | 2.26                     | 0.43              |
| 7:K:144:CYS:SG    | 7:K:309:MET:HE2  | 2.59                     | 0.43              |
| 7:K:146:ILE:CG2   | 7:K:158:VAL:H    | 2.21                     | 0.43              |
| 7:K:270:LEU:O     | 7:K:270:LEU:HD22 | 2.19                     | 0.43              |
| 13:V:139:SER:HB3  | 13:V:142:GLU:CG  | 2.45                     | 0.43              |
| 13:V:143:TYR:CE1  | 13:V:154:LYS:CG  | 3.02                     | 0.43              |
| 15:X:28:DG:H2''   | 15:X:29:DG:C8    | 2.52                     | 0.43              |
| 15:X:114:DC:H2'   | 15:X:114:DC:OP2  | 2.19                     | 0.43              |
| 16:Y:-78:DA:H2''  | 16:Y:-77:DC:C5   | 2.54                     | 0.43              |
| 1:A:33:ARG:HD3    | 1:A:37:LYS:HE2   | 1.99                     | 0.43              |
| 1:A:65:GLU:N      | 1:A:65:GLU:OE1   | 2.52                     | 0.43              |
| 4:H:31:LYS:N      | 4:H:32:PRO:HD2   | 2.33                     | 0.43              |
| 5:I:1993:CYS:SG   | 5:I:1994:HIS:N   | 2.92                     | 0.43              |
| 7:K:106:GLN:O     | 7:K:109:MET:HB3  | 2.18                     | 0.43              |
| 7:K:220:MET:CE    | 8:L:123:PRO:HD3  | 2.43                     | 0.43              |
| 7:K:261:TYR:CD1   | 7:K:267:ILE:HB   | 2.53                     | 0.43              |
| 16:Y:-107:DG:C1'  | 16:Y:-106:DA:C8  | 2.97                     | 0.43              |
| 1:A:70:ALA:O      | 1:A:73:ASP:HB2   | 2.19                     | 0.42              |
| 3:C:96:CYS:SG     | 4:D:62:LEU:CD2   | 3.07                     | 0.42              |
| 3:C:128:ARG:NH1   | 3:C:133:GLU:HB3  | 2.34                     | 0.42              |
| 7:K:15:ILE:O      | 7:K:15:ILE:HG13  | 2.18                     | 0.42              |
| 7:K:60:PHE:HB3    | 7:K:63:GLY:HA2   | 2.00                     | 0.42              |
| 7:K:67:ASN:C      | 7:K:69:ASP:N     | 2.76                     | 0.42              |
| 7:K:72:ARG:O      | 7:K:73:GLN:C     | 2.62                     | 0.42              |
| 7:K:224:LYS:CG    | 8:L:122:PHE:CE2  | 3.02                     | 0.42              |
| 7:K:358:TYR:HA    | 7:K:361:GLU:OE1  | 2.19                     | 0.42              |
| 12:T:338:ILE:HD11 | 13:V:234:TYR:HB2 | 2.01                     | 0.42              |
| 11:U:140:LEU:O    | 11:U:342:GLY:HA3 | 2.19                     | 0.42              |
| 16:Y:-21:DG:H2'   | 16:Y:-20:DT:C5   | 2.54                     | 0.42              |
| 16:Y:-14:DA:O3'   | 16:Y:-13:DT:C6   | 2.72                     | 0.42              |
| 7:K:159:PRO:HG3   | 7:K:169:ALA:HB3  | 2.01                     | 0.42              |
| 12:T:184:ASP:HB3  | 13:V:170:ARG:NH1 | 2.34                     | 0.42              |
| 13:V:57:VAL:O     | 13:V:61:LEU:HG   | 2.19                     | 0.42              |
| 13:V:238:PRO:O    | 13:V:239:GLU:C   | 2.62                     | 0.42              |
| 13:V:261:ARG:O    | 14:W:198:LYS:CD  | 2.66                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 15:X:2:DA:C2'     | 15:X:3:DG:N7     | 2.74                     | 0.42              |
| 1:A:55:VAL:HG21   | 2:B:95:VAL:HG21  | 2.01                     | 0.42              |
| 3:C:99:TYR:HA     | 4:D:95:ARG:NH2   | 2.35                     | 0.42              |
| 1:E:26:PRO:HB3    | 2:F:37:TYR:CZ    | 2.53                     | 0.42              |
| 4:H:35:ARG:HB2    | 4:H:35:ARG:HH11  | 1.80                     | 0.42              |
| 6:J:155:SER:HA    | 16:Y:-135:DC:OP1 | 2.19                     | 0.42              |
| 7:K:36:ARG:HG3    | 7:K:36:ARG:HH21  | 1.84                     | 0.42              |
| 7:K:88:PHE:CA     | 7:K:119:PHE:HD2  | 2.32                     | 0.42              |
| 7:K:121:ALA:N     | 7:K:378:THR:OG1  | 2.52                     | 0.42              |
| 7:K:220:MET:O     | 7:K:224:LYS:CG   | 2.64                     | 0.42              |
| 7:K:282:PHE:CE2   | 7:K:333:VAL:HG23 | 2.54                     | 0.42              |
| 7:K:306:PRO:HB2   | 7:K:309:MET:HB3  | 2.02                     | 0.42              |
| 7:K:315:LYS:HG3   | 7:K:346:ASP:O    | 2.19                     | 0.42              |
| 9:M:401:THR:CG2   | 9:M:402:THR:N    | 2.83                     | 0.42              |
| 10:N:249:VAL:HG12 | 10:N:256:GLY:O   | 2.19                     | 0.42              |
| 11:U:332:PRO:O    | 11:U:335:ARG:HD2 | 2.19                     | 0.42              |
| 16:Y:-20:DT:H2''  | 16:Y:-19:DG:OP2  | 2.19                     | 0.42              |
| 3:C:61:LEU:N      | 3:C:97:GLU:OE2   | 2.51                     | 0.42              |
| 1:E:34:LEU:HD13   | 1:E:43:VAL:HG13  | 2.01                     | 0.42              |
| 3:G:63:ARG:HH21   | 15:X:59:DA:C4'   | 2.31                     | 0.42              |
| 3:G:73:GLU:HA     | 4:H:23:ARG:CZ    | 2.50                     | 0.42              |
| 7:K:65:LEU:HB3    | 7:K:68:TRP:CZ3   | 2.54                     | 0.42              |
| 7:K:206:LYS:HA    | 7:K:210:CYS:SG   | 2.60                     | 0.42              |
| 7:K:330:ARG:HG2   | 7:K:351:LEU:HB2  | 2.02                     | 0.42              |
| 7:K:338:ARG:HA    | 7:K:347:VAL:HG11 | 2.00                     | 0.42              |
| 9:M:35:ALA:HB2    | 9:M:40:VAL:HG22  | 1.99                     | 0.42              |
| 11:U:150:GLY:HA2  | 11:U:296:ASN:O   | 2.19                     | 0.42              |
| 14:W:150:MET:O    | 14:W:154:LEU:HG  | 2.19                     | 0.42              |
| 15:X:7:DG:H2''    | 15:X:8:DT:H5''   | 2.00                     | 0.42              |
| 15:X:98:DT:H1'    | 15:X:99:DA:C8    | 2.55                     | 0.42              |
| 15:X:110:DC:H2''  | 15:X:111:DG:H8   | 1.82                     | 0.42              |
| 16:Y:-67:DC:H1'   | 16:Y:-66:DC:C6   | 2.55                     | 0.42              |
| 1:A:57:GLU:HG3    | 2:B:41:VAL:HG21  | 2.01                     | 0.42              |
| 1:E:67:GLY:CA     | 1:E:78:ILE:HG12  | 2.23                     | 0.42              |
| 1:E:95:LYS:HB3    | 1:E:95:LYS:NZ    | 2.35                     | 0.42              |
| 5:I:1883:PRO:HG2  | 7:K:308:GLU:HG2  | 2.00                     | 0.42              |
| 7:K:32:SER:HB2    | 7:K:54:LEU:HD21  | 2.00                     | 0.42              |
| 7:K:216:PHE:HE2   | 8:L:116:PHE:HZ   | 1.67                     | 0.42              |
| 10:P:227:CYS:HB2  | 10:P:228:PRO:HD2 | 2.02                     | 0.42              |
| 11:U:111:ASN:O    | 11:U:115:ASN:HB2 | 2.19                     | 0.42              |
| 13:V:202:LEU:HD23 | 13:V:202:LEU:HA  | 1.74                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:X:99:DA:H2''   | 15:X:100:DG:H5'   | 2.01                     | 0.42              |
| 1:A:57:GLU:CD     | 8:L:9:ARG:HH21    | 2.27                     | 0.42              |
| 1:E:66:ALA:HB2    | 1:E:83:LEU:HD23   | 2.02                     | 0.42              |
| 1:E:118:LYS:HE2   | 1:E:118:LYS:HB3   | 1.81                     | 0.42              |
| 3:G:107:THR:O     | 3:G:123:ASP:HB3   | 2.20                     | 0.42              |
| 5:I:102:HIS:CE1   | 13:V:253:LYS:HB3  | 2.55                     | 0.42              |
| 5:I:834:ARG:N     | 5:I:835:PRO:CD    | 2.82                     | 0.42              |
| 5:I:2123:VAL:HG13 | 5:I:2124:GLY:N    | 2.34                     | 0.42              |
| 7:K:36:ARG:NH2    | 7:K:36:ARG:HG3    | 2.34                     | 0.42              |
| 7:K:100:PHE:HZ    | 7:K:170:ILE:HG12  | 1.83                     | 0.42              |
| 7:K:135:TYR:HA    | 7:K:138:ASP:OD1   | 2.20                     | 0.42              |
| 9:M:401:THR:HG21  | 9:M:405:TYR:CD2   | 2.55                     | 0.42              |
| 13:V:196:TYR:HB3  | 13:V:217:VAL:CG1  | 2.49                     | 0.42              |
| 14:W:194:ILE:CG2  | 14:W:198:LYS:HD2  | 2.50                     | 0.42              |
| 15:X:112:DA:C2'   | 15:X:113:DC:C6    | 3.03                     | 0.42              |
| 16:Y:-133:DG:C2'  | 16:Y:-132:DT:C7   | 2.97                     | 0.42              |
| 16:Y:-130:DC:OP2  | 16:Y:-130:DC:C6   | 2.72                     | 0.42              |
| 1:A:56:LEU:CD1    | 2:B:67:PHE:HB2    | 2.50                     | 0.42              |
| 2:F:77:LEU:HD23   | 2:F:80:TYR:HD2    | 1.85                     | 0.42              |
| 3:G:74:ILE:HD12   | 4:H:62:LEU:CD1    | 2.49                     | 0.42              |
| 5:I:122:LYS:HE2   | 5:I:122:LYS:HA    | 2.02                     | 0.42              |
| 5:I:2088:ARG:HB2  | 5:I:2115:ILE:HB   | 2.02                     | 0.42              |
| 7:K:82:GLU:H      | 7:K:82:GLU:CD     | 2.27                     | 0.42              |
| 7:K:92:ASN:HA     | 7:K:119:PHE:O     | 2.19                     | 0.42              |
| 7:K:97:GLU:OE2    | 7:K:124:ARG:HD3   | 2.19                     | 0.42              |
| 7:K:102:PHE:HD2   | 8:L:90:GLU:HG3    | 1.85                     | 0.42              |
| 9:M:412:PRO:C     | 9:M:433:ILE:HD13  | 2.44                     | 0.42              |
| 10:R:245:HIS:C    | 10:R:247:ILE:N    | 2.78                     | 0.42              |
| 10:R:249:VAL:O    | 10:R:249:VAL:HG12 | 2.19                     | 0.42              |
| 13:V:113:HIS:CD2  | 13:V:115:ARG:HE   | 2.32                     | 0.42              |
| 16:Y:-126:DG:H2'' | 16:Y:-125:DG:H8   | 1.84                     | 0.42              |
| 3:C:120:MET:O     | 3:C:123:ASP:N     | 2.49                     | 0.42              |
| 3:G:63:ARG:HB3    | 3:G:66:PRO:HG2    | 2.00                     | 0.42              |
| 7:K:71:GLN:OE1    | 7:K:72:ARG:HG2    | 2.20                     | 0.42              |
| 7:K:106:GLN:CA    | 7:K:109:MET:HB3   | 2.46                     | 0.42              |
| 7:K:244:ILE:HD13  | 7:K:248:PHE:HE1   | 1.85                     | 0.42              |
| 7:K:319:LEU:O     | 7:K:352:PRO:HD2   | 2.20                     | 0.42              |
| 7:K:332:ARG:HE    | 7:K:336:GLU:CD    | 2.27                     | 0.42              |
| 8:L:114:ARG:NE    | 8:L:114:ARG:HA    | 2.35                     | 0.42              |
| 10:N:312:LEU:O    | 10:N:313:ASN:C    | 2.63                     | 0.42              |
| 9:O:306:MET:HE2   | 9:O:306:MET:HB2   | 1.94                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:U:326:LYS:HE2  | 11:U:328:LYS:HB2  | 2.01                     | 0.42              |
| 13:V:248:LEU:O    | 13:V:252:ARG:CZ   | 2.67                     | 0.42              |
| 14:W:195:ALA:O    | 14:W:199:GLU:HG2  | 2.19                     | 0.42              |
| 16:Y:-124:DC:H1'  | 16:Y:-123:DC:H5'  | 2.02                     | 0.42              |
| 16:Y:-6:DA:H2''   | 16:Y:-5:DT:O5'    | 2.20                     | 0.42              |
| 1:E:88:ARG:CB     | 1:E:108:LEU:HD11  | 2.49                     | 0.42              |
| 3:G:90:MET:HE2    | 3:G:90:MET:CA     | 2.48                     | 0.42              |
| 5:I:930:LEU:CD2   | 10:N:250:ILE:CD1  | 2.96                     | 0.42              |
| 6:J:162:HIS:CE1   | 15:X:137:DG:C4'   | 2.92                     | 0.42              |
| 7:K:93:ILE:O      | 7:K:122:VAL:CA    | 2.65                     | 0.42              |
| 7:K:158:VAL:HG13  | 7:K:170:ILE:HB    | 2.02                     | 0.42              |
| 7:K:201:VAL:HA    | 7:K:204:GLN:CD    | 2.45                     | 0.42              |
| 7:K:284:PRO:HG3   | 7:K:293:GLY:H     | 1.83                     | 0.42              |
| 7:K:387:HIS:O     | 7:K:391:GLU:HG3   | 2.19                     | 0.42              |
| 10:P:208:SER:C    | 10:P:210:THR:H    | 2.28                     | 0.42              |
| 11:U:275:HIS:CG   | 11:U:276:GLU:N    | 2.88                     | 0.42              |
| 15:X:87:DT:P      | 15:X:87:DT:H2'    | 2.60                     | 0.42              |
| 15:X:114:DC:C2    | 15:X:115:DA:C5    | 3.08                     | 0.42              |
| 16:Y:-24:DC:C6    | 16:Y:-24:DC:H5'   | 2.54                     | 0.42              |
| 1:A:43:ARG:HG2    | 2:B:85:THR:HB     | 2.01                     | 0.42              |
| 1:A:93:GLU:HG2    | 2:B:100:PRO:HB2   | 2.02                     | 0.42              |
| 5:I:1928:LEU:HD22 | 10:R:279:LYS:HD2  | 2.02                     | 0.42              |
| 7:K:235:ASP:OD2   | 7:K:250:LYS:HD2   | 2.20                     | 0.42              |
| 7:K:373:GLU:H     | 7:K:373:GLU:CD    | 2.26                     | 0.42              |
| 9:M:354:LEU:O     | 9:M:358:VAL:CG2   | 2.68                     | 0.42              |
| 11:U:256:ARG:O    | 11:U:257:CYS:CB   | 2.68                     | 0.42              |
| 13:V:236:ARG:HE   | 13:V:240:GLN:C    | 2.28                     | 0.42              |
| 13:V:257:ARG:O    | 13:V:261:ARG:CG   | 2.65                     | 0.42              |
| 14:W:157:THR:O    | 14:W:157:THR:HG22 | 2.20                     | 0.42              |
| 15:X:60:DA:H5''   | 15:X:60:DA:H8     | 1.84                     | 0.42              |
| 15:X:128:DC:H6    | 15:X:128:DC:C5'   | 2.33                     | 0.42              |
| 1:E:42:ARG:O      | 2:F:85:THR:OG1    | 2.20                     | 0.41              |
| 5:I:1914:LEU:HD23 | 9:M:285:LYS:HD2   | 2.01                     | 0.41              |
| 5:I:2060:HIS:HD2  | 5:I:2132:THR:HG23 | 1.78                     | 0.41              |
| 5:I:2091:GLY:O    | 15:X:56:DT:H73    | 2.20                     | 0.41              |
| 7:K:146:ILE:O     | 7:K:318:VAL:HB    | 2.20                     | 0.41              |
| 7:K:175:VAL:CG2   | 7:K:289:ILE:HG21  | 2.50                     | 0.41              |
| 7:K:234:ILE:O     | 7:K:235:ASP:OD1   | 2.37                     | 0.41              |
| 15:X:5:DA:H2''    | 15:X:6:DT:O5'     | 2.20                     | 0.41              |
| 15:X:16:DT:C7     | 15:X:16:DT:OP2    | 2.68                     | 0.41              |
| 15:X:37:DG:OP2    | 15:X:37:DG:H8     | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Y:-23:DA:H2''  | 16:Y:-22:DC:C5'   | 2.50                     | 0.41              |
| 1:A:51:TYR:OH     | 2:B:108:VAL:HA    | 2.20                     | 0.41              |
| 1:A:113:GLN:HB2   | 1:A:116:LEU:HG    | 2.02                     | 0.41              |
| 1:E:36:LYS:HA     | 1:E:36:LYS:HD3    | 1.86                     | 0.41              |
| 1:E:57:TYR:CA     | 6:J:130:ARG:HH12  | 2.22                     | 0.41              |
| 1:E:83:LEU:HD13   | 2:F:58:ILE:HG21   | 2.02                     | 0.41              |
| 1:E:88:ARG:HB3    | 1:E:108:LEU:HD11  | 2.02                     | 0.41              |
| 5:I:694:LYS:N     | 5:I:719:HIS:HD2   | 2.15                     | 0.41              |
| 7:K:120:GLN:HE21  | 7:K:120:GLN:H     | 1.65                     | 0.41              |
| 7:K:125:VAL:CG1   | 7:K:129:ALA:HB3   | 2.50                     | 0.41              |
| 7:K:185:LYS:HE2   | 7:K:185:LYS:HB3   | 1.87                     | 0.41              |
| 7:K:261:TYR:HB2   | 7:K:267:ILE:HG12  | 2.02                     | 0.41              |
| 7:K:284:PRO:HG3   | 7:K:292:MET:HA    | 2.02                     | 0.41              |
| 9:Q:237:ASP:OD1   | 9:Q:237:ASP:N     | 2.51                     | 0.41              |
| 12:T:198:ALA:H    | 12:T:201:PHE:HB3  | 1.86                     | 0.41              |
| 11:U:170:ALA:HB1  | 11:U:175:ILE:HD11 | 2.02                     | 0.41              |
| 1:A:26:PHE:CE2    | 2:B:63:VAL:CG2    | 3.03                     | 0.41              |
| 1:A:63:ILE:HG21   | 2:B:59:MET:HE1    | 2.01                     | 0.41              |
| 7:K:10:ALA:HB3    | 7:K:152:TYR:HD2   | 1.85                     | 0.41              |
| 7:K:79:PHE:O      | 7:K:80:GLY:C      | 2.63                     | 0.41              |
| 7:K:119:PHE:CD1   | 7:K:119:PHE:N     | 2.86                     | 0.41              |
| 7:K:235:ASP:CG    | 7:K:250:LYS:HB2   | 2.45                     | 0.41              |
| 7:K:276:ALA:O     | 7:K:279:GLU:HB3   | 2.21                     | 0.41              |
| 7:K:364:LYS:HE2   | 7:K:365:LEU:HD13  | 2.02                     | 0.41              |
| 9:M:317:ARG:CG    | 10:R:104:ALA:HB2  | 2.50                     | 0.41              |
| 11:U:188:TYR:CE1  | 11:U:192:ILE:HD11 | 2.55                     | 0.41              |
| 13:V:226:ARG:HA   | 13:V:229:GLN:CD   | 2.45                     | 0.41              |
| 15:X:122:DC:C2    | 15:X:123:DG:C5    | 3.08                     | 0.41              |
| 16:Y:-146:DC:C2'  | 16:Y:-145:DT:C6   | 3.03                     | 0.41              |
| 16:Y:-133:DG:H2'  | 16:Y:-132:DT:C7   | 2.48                     | 0.41              |
| 16:Y:-118:DA:H2'' | 16:Y:-117:DA:N7   | 2.35                     | 0.41              |
| 16:Y:-55:DC:H2'   | 16:Y:-54:DC:C6    | 2.55                     | 0.41              |
| 1:A:40:TYR:O      | 2:B:86:ILE:HD11   | 2.19                     | 0.41              |
| 1:A:117:LEU:HA    | 3:C:48:LEU:HD11   | 2.03                     | 0.41              |
| 2:F:77:LEU:HD23   | 2:F:77:LEU:HA     | 1.81                     | 0.41              |
| 7:K:75:TRP:HB3    | 7:K:79:PHE:CE2    | 2.56                     | 0.41              |
| 10:N:258:LEU:C    | 10:N:260:LEU:N    | 2.76                     | 0.41              |
| 10:R:112:GLU:HB2  | 10:R:265:THR:CG2  | 2.51                     | 0.41              |
| 10:R:264:ASP:OD1  | 10:R:265:THR:N    | 2.53                     | 0.41              |
| 10:R:328:THR:HG21 | 10:R:344:HIS:HB3  | 2.02                     | 0.41              |
| 15:X:87:DT:C1'    | 15:X:88:DT:H72    | 2.51                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Y:-120:DT:H1'  | 16:Y:-119:DC:C5'  | 2.47                     | 0.41              |
| 1:A:84:LEU:HD12   | 2:B:58:ILE:HD13   | 2.02                     | 0.41              |
| 1:A:101:VAL:HG11  | 4:D:98:TYR:CE2    | 2.55                     | 0.41              |
| 2:B:75:SER:HA     | 2:B:86:ILE:CG1    | 2.50                     | 0.41              |
| 2:B:106:HIS:CD2   | 2:B:106:HIS:N     | 2.88                     | 0.41              |
| 1:E:74:LYS:HD3    | 6:J:151:ARG:HD3   | 2.02                     | 0.41              |
| 5:I:128:PRO:HG3   | 13:V:218:PHE:N    | 2.36                     | 0.41              |
| 5:I:979:THR:HG23  | 5:I:980:ALA:N     | 2.36                     | 0.41              |
| 7:K:146:ILE:HG21  | 7:K:157:ILE:HG23  | 2.02                     | 0.41              |
| 7:K:162:ARG:HA    | 7:K:162:ARG:HE    | 1.85                     | 0.41              |
| 13:V:171:PHE:HZ   | 13:V:195:TYR:CD2  | 2.37                     | 0.41              |
| 15:X:114:DC:O5'   | 15:X:114:DC:H2'   | 2.21                     | 0.41              |
| 1:A:33:ARG:HA     | 1:A:36:ARG:CZ     | 2.50                     | 0.41              |
| 3:C:41:TYR:HD2    | 15:X:83:DG:OP1    | 2.04                     | 0.41              |
| 7:K:99:TYR:CE2    | 7:K:158:VAL:HG11  | 2.56                     | 0.41              |
| 9:M:270:GLU:HB3   | 9:M:276:ARG:HG3   | 2.01                     | 0.41              |
| 12:T:376:MET:HE1  | 13:V:234:TYR:CE2  | 2.56                     | 0.41              |
| 11:U:301:GLY:O    | 11:U:304:THR:OG1  | 2.38                     | 0.41              |
| 13:V:175:HIS:O    | 13:V:178:TYR:HB2  | 2.21                     | 0.41              |
| 13:V:238:PRO:C    | 13:V:242:ALA:H    | 2.28                     | 0.41              |
| 14:W:190:THR:O    | 14:W:194:ILE:HD12 | 2.21                     | 0.41              |
| 15:X:8:DT:C2'     | 15:X:9:DA:C8      | 3.02                     | 0.41              |
| 16:Y:-140:DA:C2'  | 16:Y:-139:DA:H5'' | 2.27                     | 0.41              |
| 1:A:55:VAL:O      | 1:A:59:LEU:CG     | 2.64                     | 0.41              |
| 3:C:61:LEU:HD11   | 4:D:40:ARG:NE     | 2.35                     | 0.41              |
| 1:E:18:SER:CB     | 1:E:27:VAL:H      | 2.33                     | 0.41              |
| 3:G:120:MET:HE2   | 3:G:120:MET:HB3   | 1.93                     | 0.41              |
| 7:K:135:TYR:O     | 7:K:139:ASN:N     | 2.53                     | 0.41              |
| 10:N:324:LEU:HD13 | 10:N:326:MET:CE   | 2.40                     | 0.41              |
| 14:W:151:MET:HE3  | 14:W:155:LEU:HD21 | 2.02                     | 0.41              |
| 14:W:194:ILE:CG2  | 14:W:198:LYS:HE2  | 2.50                     | 0.41              |
| 15:X:25:DC:H1'    | 15:X:26:DC:C2     | 2.55                     | 0.41              |
| 1:A:63:ILE:HG23   | 1:A:64:LEU:H      | 1.86                     | 0.41              |
| 3:C:124:ILE:HG13  | 4:D:50:ILE:HD12   | 2.02                     | 0.41              |
| 1:E:26:PRO:HG3    | 2:F:37:TYR:CE2    | 2.56                     | 0.41              |
| 1:E:31:HIS:CE1    | 1:E:35:ARG:HH11   | 2.38                     | 0.41              |
| 1:E:47:ALA:N      | 1:E:48:PRO:CD     | 2.84                     | 0.41              |
| 3:G:107:THR:HG21  | 3:G:119:ILE:HD12  | 2.03                     | 0.41              |
| 4:H:89:ALA:O      | 4:H:93:GLN:HG2    | 2.20                     | 0.41              |
| 5:I:120:SER:CB    | 13:V:233:LEU:HD12 | 2.44                     | 0.41              |
| 5:I:128:PRO:HG3   | 13:V:217:VAL:C    | 2.45                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:J:177:LYS:HA    | 6:J:180:GLU:HG2   | 2.02                     | 0.41              |
| 9:M:416:LEU:HD22  | 9:M:433:ILE:HG12  | 2.02                     | 0.41              |
| 13:V:236:ARG:HH21 | 13:V:241:VAL:HA   | 1.83                     | 0.41              |
| 15:X:36:DG:H1'    | 15:X:37:DG:C8     | 2.56                     | 0.41              |
| 15:X:112:DA:C2'   | 15:X:113:DC:H6    | 2.34                     | 0.41              |
| 16:Y:-49:DA:H2''  | 16:Y:-48:DG:N7    | 2.36                     | 0.41              |
| 1:A:33:ARG:HG2    | 1:A:37:LYS:HZ1    | 1.84                     | 0.41              |
| 1:A:63:ILE:O      | 1:A:64:LEU:C      | 2.63                     | 0.41              |
| 2:B:90:GLU:CA     | 2:B:93:THR:HG22   | 2.47                     | 0.41              |
| 3:C:48:LEU:HA     | 3:C:51:ILE:HD12   | 2.02                     | 0.41              |
| 2:F:34:TYR:CE1    | 2:F:63:VAL:HG11   | 2.56                     | 0.41              |
| 5:I:124:LEU:N     | 5:I:125:PRO:HD3   | 2.35                     | 0.41              |
| 5:I:895:MET:O     | 5:I:898:ARG:HB2   | 2.21                     | 0.41              |
| 5:I:1886:LEU:CD1  | 7:K:311:PRO:HB2   | 2.49                     | 0.41              |
| 5:I:1941:PRO:HG2  | 5:I:1945:HIS:CD2  | 2.56                     | 0.41              |
| 7:K:110:ASN:HB2   | 7:K:387:HIS:HD2   | 1.86                     | 0.41              |
| 7:K:226:LYS:HB3   | 7:K:226:LYS:HE3   | 1.62                     | 0.41              |
| 7:K:385:ASN:O     | 7:K:386:GLY:C     | 2.62                     | 0.41              |
| 9:M:255:ASP:C     | 9:M:257:LEU:N     | 2.78                     | 0.41              |
| 10:N:22:ILE:N     | 10:N:22:ILE:HD12  | 2.36                     | 0.41              |
| 10:P:19:ILE:HG13  | 9:Q:287:ILE:HG21  | 2.02                     | 0.41              |
| 14:W:66:ILE:HD12  | 14:W:86:TYR:CG    | 2.55                     | 0.41              |
| 14:W:140:ASP:OD1  | 14:W:141:GLU:N    | 2.47                     | 0.41              |
| 16:Y:-17:DC:H6    | 16:Y:-17:DC:H2'   | 1.78                     | 0.41              |
| 1:A:59:LEU:HD13   | 2:B:66:ILE:HG21   | 1.98                     | 0.41              |
| 2:B:122:LYS:C     | 8:L:2:VAL:HG12    | 2.45                     | 0.41              |
| 5:I:815:ILE:HG23  | 5:I:816:GLU:N     | 2.36                     | 0.41              |
| 5:I:2044:LYS:NZ   | 5:I:2173:GLU:CD   | 2.77                     | 0.41              |
| 5:I:2131:ASP:OD2  | 5:I:2132:THR:HG23 | 2.21                     | 0.41              |
| 7:K:106:GLN:HA    | 7:K:109:MET:CB    | 2.50                     | 0.41              |
| 7:K:120:GLN:H     | 7:K:379:ARG:HH22  | 1.68                     | 0.41              |
| 7:K:183:HIS:CE1   | 7:K:187:ILE:HG13  | 2.56                     | 0.41              |
| 7:K:380:GLU:HG3   | 7:K:380:GLU:H     | 1.52                     | 0.41              |
| 11:S:252:ASN:HA   | 11:S:255:PHE:CE1  | 2.55                     | 0.41              |
| 13:V:228:GLU:O    | 13:V:231:GLU:N    | 2.50                     | 0.41              |
| 14:W:194:ILE:HG23 | 14:W:198:LYS:CE   | 2.50                     | 0.41              |
| 15:X:60:DA:H5''   | 15:X:60:DA:C8     | 2.56                     | 0.41              |
| 16:Y:-116:DT:C6   | 16:Y:-116:DT:H5'  | 2.54                     | 0.41              |
| 16:Y:-91:DC:H2''  | 16:Y:-90:DT:OP2   | 2.21                     | 0.41              |
| 16:Y:-33:DG:H2'   | 16:Y:-32:DT:H71   | 2.03                     | 0.41              |
| 16:Y:-1:DG:H1'    | 16:Y:0:DT:H5''    | 2.03                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:98:LEU:HD13  | 2:B:98:LEU:HA     | 1.94                     | 0.40              |
| 2:B:112:THR:CG2  | 13:V:61:LEU:HD21  | 2.51                     | 0.40              |
| 5:I:888:MET:HE3  | 5:I:888:MET:HB2   | 1.97                     | 0.40              |
| 7:K:72:ARG:NH1   | 7:K:72:ARG:HA     | 2.36                     | 0.40              |
| 7:K:98:PRO:O     | 7:K:99:TYR:C      | 2.64                     | 0.40              |
| 7:K:123:LEU:HD13 | 7:K:372:PHE:CD1   | 2.56                     | 0.40              |
| 7:K:335:SER:HA   | 7:K:338:ARG:NE    | 2.31                     | 0.40              |
| 9:Q:129:GLU:HG2  | 9:Q:195:ALA:HB3   | 2.03                     | 0.40              |
| 9:Q:137:GLU:O    | 9:Q:159:ILE:HA    | 2.22                     | 0.40              |
| 12:T:157:LEU:O   | 12:T:396:GLY:HA3  | 2.21                     | 0.40              |
| 13:V:224:ARG:HE  | 13:V:224:ARG:HB2  | 1.50                     | 0.40              |
| 15:X:87:DT:H2'   | 15:X:87:DT:OP2    | 2.21                     | 0.40              |
| 16:Y:-15:DC:H6   | 16:Y:-15:DC:H5''  | 1.86                     | 0.40              |
| 16:Y:-11:DT:H2'' | 16:Y:-10:DA:OP2   | 2.21                     | 0.40              |
| 3:C:73:GLU:HB3   | 4:D:25:ASN:HD22   | 1.86                     | 0.40              |
| 3:G:110:CYS:HB2  | 3:G:123:ASP:CB    | 2.48                     | 0.40              |
| 4:H:70:VAL:O     | 4:H:74:GLU:HG3    | 2.20                     | 0.40              |
| 5:I:903:HIS:CG   | 5:I:904:PRO:HD2   | 2.56                     | 0.40              |
| 7:K:59:PRO:HA    | 7:K:67:ASN:HD22   | 1.85                     | 0.40              |
| 7:K:115:GLU:HA   | 7:K:118:GLN:CD    | 2.45                     | 0.40              |
| 7:K:171:ILE:HD11 | 7:K:300:TYR:HD1   | 1.87                     | 0.40              |
| 9:M:28:GLU:H     | 9:M:28:GLU:CD     | 2.29                     | 0.40              |
| 9:M:389:GLU:HG2  | 9:M:427:LYS:HB2   | 2.02                     | 0.40              |
| 9:M:416:LEU:HD22 | 9:M:433:ILE:HG13  | 2.02                     | 0.40              |
| 10:P:68:ILE:HD13 | 10:P:68:ILE:N     | 2.33                     | 0.40              |
| 10:R:207:ARG:HD3 | 10:R:207:ARG:H    | 1.87                     | 0.40              |
| 10:R:211:ARG:HB3 | 10:R:211:ARG:CZ   | 2.51                     | 0.40              |
| 11:U:256:ARG:O   | 11:U:257:CYS:HB3  | 2.21                     | 0.40              |
| 13:V:128:ARG:HG3 | 13:V:129:PHE:HD1  | 1.84                     | 0.40              |
| 15:X:10:DT:C2    | 15:X:11:DA:N7     | 2.89                     | 0.40              |
| 15:X:47:DC:H2''  | 15:X:48:DC:C5     | 2.56                     | 0.40              |
| 1:A:52:LEU:HD11  | 1:A:56:LEU:HD11   | 2.03                     | 0.40              |
| 5:I:887:PHE:O    | 5:I:890:VAL:HG22  | 2.20                     | 0.40              |
| 7:K:4:LEU:HB2    | 7:K:93:ILE:CG1    | 2.50                     | 0.40              |
| 7:K:36:ARG:HA    | 7:K:36:ARG:HE     | 1.82                     | 0.40              |
| 7:K:98:PRO:HG2   | 7:K:101:ASN:HB2   | 2.02                     | 0.40              |
| 7:K:156:HIS:HA   | 7:K:171:ILE:O     | 2.20                     | 0.40              |
| 7:K:165:LYS:HZ2  | 7:K:167:LYS:CD    | 2.32                     | 0.40              |
| 10:R:144:GLU:N   | 10:R:162:THR:OG1  | 2.55                     | 0.40              |
| 10:R:324:LEU:CD1 | 10:R:326:MET:HE3  | 2.51                     | 0.40              |
| 13:V:250:GLU:C   | 13:V:254:ILE:HG23 | 2.43                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 15:X:115:DA:H2''  | 15:X:116:DA:H8   | 1.85                     | 0.40              |
| 1:E:62:ILE:HD12   | 2:F:62:PHE:CZ    | 2.56                     | 0.40              |
| 5:I:154:GLU:OE2   | 5:I:158:LYS:NZ   | 2.41                     | 0.40              |
| 7:K:120:GLN:HA    | 7:K:378:THR:HG21 | 2.01                     | 0.40              |
| 7:K:169:ALA:O     | 7:K:301:SER:OG   | 2.32                     | 0.40              |
| 7:K:214:GLN:NE2   | 7:K:331:ASP:OD2  | 2.54                     | 0.40              |
| 7:K:224:LYS:HG2   | 8:L:122:PHE:CE2  | 2.56                     | 0.40              |
| 10:P:147:ILE:HD12 | 10:P:148:ASP:N   | 2.36                     | 0.40              |
| 15:X:28:DG:C2'    | 15:X:29:DG:C8    | 3.04                     | 0.40              |
| 15:X:101:DA:C2'   | 15:X:102:DG:C8   | 3.04                     | 0.40              |
| 16:Y:-61:DT:H2''  | 16:Y:-60:DT:C6   | 2.57                     | 0.40              |
| 2:B:67:PHE:C      | 2:B:67:PHE:CD1   | 3.00                     | 0.40              |
| 1:E:70:ALA:HA     | 1:E:82:HIS:ND1   | 2.37                     | 0.40              |
| 3:G:68:GLN:OE1    | 3:G:72:ARG:NH2   | 2.49                     | 0.40              |
| 3:G:74:ILE:CD1    | 4:H:62:LEU:HB3   | 2.48                     | 0.40              |
| 3:G:83:ARG:HB2    | 4:H:80:THR:HG22  | 2.02                     | 0.40              |
| 4:H:26:ILE:HG13   | 4:H:26:ILE:O     | 2.20                     | 0.40              |
| 5:I:105:GLU:OE2   | 13:V:246:TYR:OH  | 2.35                     | 0.40              |
| 7:K:113:LEU:HD12  | 7:K:114:PHE:CD1  | 2.56                     | 0.40              |
| 7:K:377:VAL:HG22  | 7:K:389:VAL:CG2  | 2.52                     | 0.40              |
| 9:O:334:GLY:O     | 9:O:348:HIS:N    | 2.53                     | 0.40              |
| 10:R:116:THR:HG23 | 10:R:311:PHE:CE1 | 2.56                     | 0.40              |
| 12:T:353:GLY:N    | 20:T:501:ATP:O2A | 2.49                     | 0.40              |
| 14:W:188:LYS:C    | 14:W:188:LYS:HD3 | 2.47                     | 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     | 106/130 (82%) | 97 (92%) | 9 (8%)  | 0        | <b>100</b> <b>100</b> |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | E     | 103/130 (79%)   | 93 (90%)   | 10 (10%) | 0        | 100         | 100 |
| 2   | B     | 94/126 (75%)    | 87 (93%)   | 7 (7%)   | 0        | 100         | 100 |
| 2   | F     | 92/126 (73%)    | 88 (96%)   | 2 (2%)   | 2 (2%)   | 5           | 29  |
| 3   | C     | 93/136 (68%)    | 91 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 3   | G     | 95/136 (70%)    | 91 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 4   | D     | 79/103 (77%)    | 78 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 4   | H     | 78/103 (76%)    | 72 (92%)   | 6 (8%)   | 0        | 100         | 100 |
| 5   | I     | 858/3230 (27%)  | 792 (92%)  | 63 (7%)  | 3 (0%)   | 36          | 68  |
| 6   | J     | 158/364 (43%)   | 145 (92%)  | 13 (8%)  | 0        | 100         | 100 |
| 7   | K     | 392/396 (99%)   | 295 (75%)  | 84 (21%) | 13 (3%)  | 3           | 21  |
| 8   | L     | 109/154 (71%)   | 96 (88%)   | 13 (12%) | 0        | 100         | 100 |
| 9   | M     | 412/456 (90%)   | 395 (96%)  | 16 (4%)  | 1 (0%)   | 43          | 73  |
| 9   | O     | 431/456 (94%)   | 409 (95%)  | 19 (4%)  | 3 (1%)   | 18          | 52  |
| 9   | Q     | 438/456 (96%)   | 417 (95%)  | 20 (5%)  | 1 (0%)   | 43          | 73  |
| 10  | N     | 405/463 (88%)   | 386 (95%)  | 19 (5%)  | 0        | 100         | 100 |
| 10  | P     | 423/463 (91%)   | 396 (94%)  | 26 (6%)  | 1 (0%)   | 43          | 73  |
| 10  | R     | 420/463 (91%)   | 393 (94%)  | 26 (6%)  | 1 (0%)   | 43          | 73  |
| 11  | S     | 373/375 (100%)  | 366 (98%)  | 7 (2%)   | 0        | 100         | 100 |
| 11  | U     | 355/375 (95%)   | 325 (92%)  | 29 (8%)  | 1 (0%)   | 36          | 68  |
| 12  | T     | 399/429 (93%)   | 381 (96%)  | 18 (4%)  | 0        | 100         | 100 |
| 13  | V     | 200/467 (43%)   | 178 (89%)  | 19 (10%) | 3 (2%)   | 8           | 37  |
| 14  | W     | 185/227 (82%)   | 182 (98%)  | 2 (1%)   | 1 (0%)   | 24          | 59  |
| All | All   | 6298/9764 (64%) | 5853 (93%) | 415 (7%) | 30 (0%)  | 26          | 59  |

All (30) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | I     | 820 | GLU  |
| 7   | K     | 89  | LEU  |
| 7   | K     | 103 | THR  |
| 7   | K     | 120 | GLN  |
| 7   | K     | 376 | VAL  |
| 7   | K     | 377 | VAL  |
| 9   | O     | 264 | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | U     | 257  | CYS  |
| 13  | V     | 207  | ALA  |
| 13  | V     | 238  | PRO  |
| 13  | V     | 239  | GLU  |
| 2   | F     | 30   | ARG  |
| 7   | K     | 68   | TRP  |
| 7   | K     | 173  | ILE  |
| 7   | K     | 199  | THR  |
| 7   | K     | 231  | THR  |
| 9   | O     | 17   | SER  |
| 9   | O     | 266  | PRO  |
| 10  | P     | 21   | ARG  |
| 2   | F     | 29   | SER  |
| 7   | K     | 232  | VAL  |
| 14  | W     | 171  | GLU  |
| 5   | I     | 1993 | CYS  |
| 9   | M     | 37   | SER  |
| 7   | K     | 269  | ARG  |
| 9   | Q     | 256  | ILE  |
| 7   | K     | 175  | VAL  |
| 7   | K     | 305  | LEU  |
| 10  | R     | 44   | GLN  |
| 5   | I     | 133  | 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     | 84/99 (85%)  | 63 (75%)  | 21 (25%) | 0           | 3  |
| 1   | E     | 82/99 (83%)  | 68 (83%)  | 14 (17%) | 2           | 11 |
| 2   | B     | 83/106 (78%) | 67 (81%)  | 16 (19%) | 1           | 8  |
| 2   | F     | 81/106 (76%) | 73 (90%)  | 8 (10%)  | 7           | 31 |
| 3   | C     | 82/111 (74%) | 69 (84%)  | 13 (16%) | 2           | 13 |
| 3   | G     | 85/111 (77%) | 77 (91%)  | 8 (9%)   | 8           | 33 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |     |
|-----|-------|-----------------|------------|-----------|-------------|-----|
| 4   | D     | 66/79 (84%)     | 66 (100%)  | 0         | 100         | 100 |
| 4   | H     | 65/79 (82%)     | 54 (83%)   | 11 (17%)  | 2           | 11  |
| 5   | I     | 775/2721 (28%)  | 772 (100%) | 3 (0%)    | 84          | 86  |
| 6   | J     | 148/312 (47%)   | 147 (99%)  | 1 (1%)    | 76          | 83  |
| 7   | K     | 359/361 (99%)   | 236 (66%)  | 123 (34%) | 0           | 0   |
| 8   | L     | 98/133 (74%)    | 98 (100%)  | 0         | 100         | 100 |
| 9   | M     | 353/387 (91%)   | 351 (99%)  | 2 (1%)    | 78          | 84  |
| 9   | O     | 364/387 (94%)   | 345 (95%)  | 19 (5%)   | 21          | 54  |
| 9   | Q     | 366/387 (95%)   | 338 (92%)  | 28 (8%)   | 12          | 41  |
| 10  | N     | 347/390 (89%)   | 343 (99%)  | 4 (1%)    | 63          | 79  |
| 10  | P     | 352/390 (90%)   | 325 (92%)  | 27 (8%)   | 12          | 41  |
| 10  | R     | 358/390 (92%)   | 323 (90%)  | 35 (10%)  | 7           | 31  |
| 11  | S     | 318/318 (100%)  | 317 (100%) | 1 (0%)    | 86          | 88  |
| 11  | U     | 305/318 (96%)   | 292 (96%)  | 13 (4%)   | 26          | 59  |
| 12  | T     | 346/364 (95%)   | 339 (98%)  | 7 (2%)    | 48          | 72  |
| 13  | V     | 183/400 (46%)   | 124 (68%)  | 59 (32%)  | 0           | 1   |
| 14  | W     | 168/203 (83%)   | 165 (98%)  | 3 (2%)    | 51          | 74  |
| All | All   | 5468/8251 (66%) | 5052 (92%) | 416 (8%)  | 14          | 42  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 12  | ARG  |
| 1   | A     | 21  | ARG  |
| 1   | A     | 36  | ARG  |
| 1   | A     | 37  | LYS  |
| 1   | A     | 42  | GLU  |
| 1   | A     | 44  | VAL  |
| 1   | A     | 52  | LEU  |
| 1   | A     | 59  | LEU  |
| 1   | A     | 65  | GLU  |
| 1   | A     | 66  | LEU  |
| 1   | A     | 72  | ARG  |
| 1   | A     | 78  | ARG  |
| 1   | A     | 80  | ILE  |
| 1   | A     | 82  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 85  | GLN  |
| 1   | A     | 92  | GLU  |
| 1   | A     | 96  | LYS  |
| 1   | A     | 102 | THR  |
| 1   | A     | 103 | ILE  |
| 1   | A     | 109 | LEU  |
| 1   | A     | 115 | VAL  |
| 2   | B     | 28  | ARG  |
| 2   | B     | 36  | VAL  |
| 2   | B     | 46  | HIS  |
| 2   | B     | 60  | ASN  |
| 2   | B     | 68  | GLU  |
| 2   | B     | 77  | LEU  |
| 2   | B     | 85  | THR  |
| 2   | B     | 88  | SER  |
| 2   | B     | 89  | ARG  |
| 2   | B     | 98  | LEU  |
| 2   | B     | 99  | LEU  |
| 2   | B     | 102 | GLU  |
| 2   | B     | 103 | LEU  |
| 2   | B     | 106 | HIS  |
| 2   | B     | 113 | LYS  |
| 2   | B     | 117 | LYS  |
| 3   | C     | 42  | ARG  |
| 3   | C     | 48  | LEU  |
| 3   | C     | 56  | LYS  |
| 3   | C     | 59  | GLU  |
| 3   | C     | 64  | LYS  |
| 3   | C     | 76  | GLN  |
| 3   | C     | 77  | ASP  |
| 3   | C     | 79  | LYS  |
| 3   | C     | 82  | LEU  |
| 3   | C     | 115 | LYS  |
| 3   | C     | 120 | MET  |
| 3   | C     | 122 | LYS  |
| 3   | C     | 129 | ARG  |
| 1   | E     | 15  | LYS  |
| 1   | E     | 25  | PHE  |
| 1   | E     | 35  | ARG  |
| 1   | E     | 42  | ARG  |
| 1   | E     | 64  | GLU  |
| 1   | E     | 74  | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 75   | LYS  |
| 1   | E     | 76   | THR  |
| 1   | E     | 81   | ARG  |
| 1   | E     | 90   | ASP  |
| 1   | E     | 92   | GLU  |
| 1   | E     | 95   | LYS  |
| 1   | E     | 101  | THR  |
| 1   | E     | 111  | ILE  |
| 2   | F     | 28   | ARG  |
| 2   | F     | 30   | ARG  |
| 2   | F     | 31   | LYS  |
| 2   | F     | 45   | VAL  |
| 2   | F     | 60   | ASN  |
| 2   | F     | 79   | HIS  |
| 2   | F     | 86   | ILE  |
| 2   | F     | 102  | GLU  |
| 3   | G     | 56   | LYS  |
| 3   | G     | 59   | GLU  |
| 3   | G     | 76   | GLN  |
| 3   | G     | 77   | ASP  |
| 3   | G     | 117  | VAL  |
| 3   | G     | 119  | ILE  |
| 3   | G     | 129  | ARG  |
| 3   | G     | 134  | ARG  |
| 4   | H     | 25   | ASN  |
| 4   | H     | 44   | LYS  |
| 4   | H     | 46   | ILE  |
| 4   | H     | 49   | LEU  |
| 4   | H     | 50   | ILE  |
| 4   | H     | 59   | LYS  |
| 4   | H     | 62   | LEU  |
| 4   | H     | 79   | LYS  |
| 4   | H     | 84   | MET  |
| 4   | H     | 91   | LYS  |
| 4   | H     | 97   | LEU  |
| 5   | I     | 239  | GLN  |
| 5   | I     | 241  | GLU  |
| 5   | I     | 2029 | ARG  |
| 6   | J     | 219  | VAL  |
| 7   | K     | 1    | MET  |
| 7   | K     | 5    | VAL  |
| 7   | K     | 6    | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | K     | 7   | ASP  |
| 7   | K     | 8   | ASN  |
| 7   | K     | 14  | LYS  |
| 7   | K     | 17  | TYR  |
| 7   | K     | 20  | GLU  |
| 7   | K     | 23  | SER  |
| 7   | K     | 24  | VAL  |
| 7   | K     | 25  | ILE  |
| 7   | K     | 33  | LYS  |
| 7   | K     | 34  | THR  |
| 7   | K     | 36  | ARG  |
| 7   | K     | 38  | LYS  |
| 7   | K     | 52  | SER  |
| 7   | K     | 62  | LYS  |
| 7   | K     | 65  | LEU  |
| 7   | K     | 66  | VAL  |
| 7   | K     | 67  | ASN  |
| 7   | K     | 69  | ASP  |
| 7   | K     | 70  | VAL  |
| 7   | K     | 71  | GLN  |
| 7   | K     | 72  | ARG  |
| 7   | K     | 81  | LYS  |
| 7   | K     | 82  | GLU  |
| 7   | K     | 83  | MET  |
| 7   | K     | 86  | VAL  |
| 7   | K     | 87  | ASP  |
| 7   | K     | 89  | LEU  |
| 7   | K     | 94  | ILE  |
| 7   | K     | 95  | ILE  |
| 7   | K     | 97  | GLU  |
| 7   | K     | 107 | GLU  |
| 7   | K     | 115 | GLU  |
| 7   | K     | 119 | PHE  |
| 7   | K     | 120 | GLN  |
| 7   | K     | 124 | ARG  |
| 7   | K     | 133 | HIS  |
| 7   | K     | 138 | ASP  |
| 7   | K     | 146 | ILE  |
| 7   | K     | 153 | SER  |
| 7   | K     | 154 | PHE  |
| 7   | K     | 155 | THR  |
| 7   | K     | 158 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | K     | 164 | LYS  |
| 7   | K     | 166 | LYS  |
| 7   | K     | 167 | LYS  |
| 7   | K     | 168 | GLU  |
| 7   | K     | 170 | ILE  |
| 7   | K     | 174 | ASN  |
| 7   | K     | 178 | LYS  |
| 7   | K     | 181 | THR  |
| 7   | K     | 183 | HIS  |
| 7   | K     | 185 | LYS  |
| 7   | K     | 186 | GLU  |
| 7   | K     | 190 | TYR  |
| 7   | K     | 192 | GLN  |
| 7   | K     | 193 | LEU  |
| 7   | K     | 197 | ASP  |
| 7   | K     | 198 | GLU  |
| 7   | K     | 201 | VAL  |
| 7   | K     | 202 | ILE  |
| 7   | K     | 205 | VAL  |
| 7   | K     | 206 | LYS  |
| 7   | K     | 207 | GLU  |
| 7   | K     | 209 | VAL  |
| 7   | K     | 213 | SER  |
| 7   | K     | 214 | GLN  |
| 7   | K     | 217 | TYR  |
| 7   | K     | 218 | ARG  |
| 7   | K     | 222 | ILE  |
| 7   | K     | 224 | LYS  |
| 7   | K     | 225 | LEU  |
| 7   | K     | 226 | LYS  |
| 7   | K     | 228 | GLU  |
| 7   | K     | 229 | GLU  |
| 7   | K     | 233 | MET  |
| 7   | K     | 237 | VAL  |
| 7   | K     | 238 | LEU  |
| 7   | K     | 242 | SER  |
| 7   | K     | 244 | ILE  |
| 7   | K     | 266 | GLN  |
| 7   | K     | 269 | ARG  |
| 7   | K     | 270 | LEU  |
| 7   | K     | 273 | GLU  |
| 7   | K     | 274 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | K     | 280 | ILE  |
| 7   | K     | 287 | ILE  |
| 7   | K     | 289 | ILE  |
| 7   | K     | 291 | GLU  |
| 7   | K     | 292 | MET  |
| 7   | K     | 294 | ILE  |
| 7   | K     | 299 | VAL  |
| 7   | K     | 304 | ASN  |
| 7   | K     | 305 | LEU  |
| 7   | K     | 309 | MET  |
| 7   | K     | 310 | GLN  |
| 7   | K     | 312 | HIS  |
| 7   | K     | 314 | PHE  |
| 7   | K     | 315 | LYS  |
| 7   | K     | 325 | LEU  |
| 7   | K     | 326 | PHE  |
| 7   | K     | 330 | ARG  |
| 7   | K     | 331 | ASP  |
| 7   | K     | 335 | SER  |
| 7   | K     | 336 | GLU  |
| 7   | K     | 340 | LEU  |
| 7   | K     | 347 | VAL  |
| 7   | K     | 350 | VAL  |
| 7   | K     | 356 | ILE  |
| 7   | K     | 364 | LYS  |
| 7   | K     | 365 | LEU  |
| 7   | K     | 366 | ILE  |
| 7   | K     | 368 | GLU  |
| 7   | K     | 371 | ASP  |
| 7   | K     | 374 | ASP  |
| 7   | K     | 378 | THR  |
| 7   | K     | 379 | ARG  |
| 7   | K     | 380 | GLU  |
| 7   | K     | 383 | GLU  |
| 7   | K     | 385 | ASN  |
| 7   | K     | 391 | GLU  |
| 9   | M     | 192 | TYR  |
| 9   | M     | 317 | ARG  |
| 10  | N     | 192 | VAL  |
| 10  | N     | 194 | THR  |
| 10  | N     | 380 | VAL  |
| 10  | N     | 407 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | O     | 17  | SER  |
| 9   | O     | 18  | HIS  |
| 9   | O     | 21  | VAL  |
| 9   | O     | 37  | SER  |
| 9   | O     | 109 | THR  |
| 9   | O     | 137 | GLU  |
| 9   | O     | 194 | GLU  |
| 9   | O     | 216 | GLU  |
| 9   | O     | 228 | VAL  |
| 9   | O     | 265 | LYS  |
| 9   | O     | 266 | PRO  |
| 9   | O     | 278 | GLU  |
| 9   | O     | 315 | LEU  |
| 9   | O     | 319 | LEU  |
| 9   | O     | 342 | GLU  |
| 9   | O     | 378 | ARG  |
| 9   | O     | 391 | LEU  |
| 9   | O     | 407 | VAL  |
| 9   | O     | 428 | GLU  |
| 10  | P     | 18  | ARG  |
| 10  | P     | 21  | ARG  |
| 10  | P     | 28  | ILE  |
| 10  | P     | 59  | VAL  |
| 10  | P     | 62  | MET  |
| 10  | P     | 68  | ILE  |
| 10  | P     | 103 | ILE  |
| 10  | P     | 108 | ILE  |
| 10  | P     | 116 | THR  |
| 10  | P     | 147 | ILE  |
| 10  | P     | 236 | LYS  |
| 10  | P     | 257 | PHE  |
| 10  | P     | 262 | SER  |
| 10  | P     | 267 | GLU  |
| 10  | P     | 268 | ILE  |
| 10  | P     | 286 | GLU  |
| 10  | P     | 316 | LEU  |
| 10  | P     | 323 | VAL  |
| 10  | P     | 324 | LEU  |
| 10  | P     | 328 | THR  |
| 10  | P     | 348 | ILE  |
| 10  | P     | 373 | ILE  |
| 10  | P     | 405 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | P     | 407 | THR  |
| 10  | P     | 422 | GLN  |
| 10  | P     | 424 | ASP  |
| 10  | P     | 429 | VAL  |
| 9   | Q     | 21  | VAL  |
| 9   | Q     | 40  | VAL  |
| 9   | Q     | 52  | ILE  |
| 9   | Q     | 91  | VAL  |
| 9   | Q     | 113 | MET  |
| 9   | Q     | 138 | LEU  |
| 9   | Q     | 165 | LYS  |
| 9   | Q     | 180 | LEU  |
| 9   | Q     | 181 | GLN  |
| 9   | Q     | 185 | VAL  |
| 9   | Q     | 211 | THR  |
| 9   | Q     | 212 | GLU  |
| 9   | Q     | 215 | LEU  |
| 9   | Q     | 237 | ASP  |
| 9   | Q     | 262 | GLN  |
| 9   | Q     | 265 | LYS  |
| 9   | Q     | 268 | LYS  |
| 9   | Q     | 270 | GLU  |
| 9   | Q     | 274 | LYS  |
| 9   | Q     | 308 | ASP  |
| 9   | Q     | 316 | HIS  |
| 9   | Q     | 326 | ILE  |
| 9   | Q     | 352 | LEU  |
| 9   | Q     | 384 | ILE  |
| 9   | Q     | 391 | LEU  |
| 9   | Q     | 409 | LEU  |
| 9   | Q     | 430 | VAL  |
| 9   | Q     | 450 | GLN  |
| 10  | R     | 59  | VAL  |
| 10  | R     | 92  | GLN  |
| 10  | R     | 166 | THR  |
| 10  | R     | 168 | MET  |
| 10  | R     | 201 | LYS  |
| 10  | R     | 207 | ARG  |
| 10  | R     | 215 | TYR  |
| 10  | R     | 225 | VAL  |
| 10  | R     | 238 | VAL  |
| 10  | R     | 246 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | R     | 250 | ILE  |
| 10  | R     | 255 | GLN  |
| 10  | R     | 258 | LEU  |
| 10  | R     | 267 | GLU  |
| 10  | R     | 268 | ILE  |
| 10  | R     | 269 | LYS  |
| 10  | R     | 279 | LYS  |
| 10  | R     | 285 | GLU  |
| 10  | R     | 286 | GLU  |
| 10  | R     | 306 | ILE  |
| 10  | R     | 308 | SER  |
| 10  | R     | 316 | LEU  |
| 10  | R     | 323 | VAL  |
| 10  | R     | 324 | LEU  |
| 10  | R     | 346 | ILE  |
| 10  | R     | 351 | LEU  |
| 10  | R     | 353 | ARG  |
| 10  | R     | 374 | ARG  |
| 10  | R     | 392 | ARG  |
| 10  | R     | 395 | LEU  |
| 10  | R     | 407 | THR  |
| 10  | R     | 422 | GLN  |
| 10  | R     | 423 | VAL  |
| 10  | R     | 436 | GLU  |
| 10  | R     | 444 | LYS  |
| 11  | S     | 180 | LEU  |
| 12  | T     | 10  | GLU  |
| 12  | T     | 24  | ARG  |
| 12  | T     | 70  | ILE  |
| 12  | T     | 82  | MET  |
| 12  | T     | 140 | MET  |
| 12  | T     | 317 | LEU  |
| 12  | T     | 389 | ARG  |
| 11  | U     | 54  | VAL  |
| 11  | U     | 85  | ILE  |
| 11  | U     | 101 | HIS  |
| 11  | U     | 104 | LEU  |
| 11  | U     | 107 | GLU  |
| 11  | U     | 151 | ILE  |
| 11  | U     | 161 | HIS  |
| 11  | U     | 163 | VAL  |
| 11  | U     | 226 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | U     | 297 | THR  |
| 11  | U     | 306 | TYR  |
| 11  | U     | 326 | LYS  |
| 11  | U     | 330 | ILE  |
| 13  | V     | 51  | GLU  |
| 13  | V     | 53  | MET  |
| 13  | V     | 56  | GLU  |
| 13  | V     | 65  | LYS  |
| 13  | V     | 90  | LYS  |
| 13  | V     | 91  | LYS  |
| 13  | V     | 93  | ARG  |
| 13  | V     | 96  | LYS  |
| 13  | V     | 114 | TRP  |
| 13  | V     | 119 | GLU  |
| 13  | V     | 120 | GLU  |
| 13  | V     | 131 | LYS  |
| 13  | V     | 134 | GLN  |
| 13  | V     | 135 | VAL  |
| 13  | V     | 137 | VAL  |
| 13  | V     | 141 | GLN  |
| 13  | V     | 145 | LEU  |
| 13  | V     | 147 | LEU  |
| 13  | V     | 153 | THR  |
| 13  | V     | 156 | GLU  |
| 13  | V     | 169 | LEU  |
| 13  | V     | 174 | ILE  |
| 13  | V     | 182 | GLN  |
| 13  | V     | 189 | GLU  |
| 13  | V     | 190 | ASP  |
| 13  | V     | 202 | LEU  |
| 13  | V     | 205 | VAL  |
| 13  | V     | 206 | ARG  |
| 13  | V     | 208 | VAL  |
| 13  | V     | 214 | LYS  |
| 13  | V     | 217 | VAL  |
| 13  | V     | 218 | PHE  |
| 13  | V     | 219 | ASP  |
| 13  | V     | 222 | HIS  |
| 13  | V     | 223 | GLU  |
| 13  | V     | 224 | ARG  |
| 13  | V     | 225 | ARG  |
| 13  | V     | 226 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | V     | 230 | LEU  |
| 13  | V     | 231 | GLU  |
| 13  | V     | 232 | ARG  |
| 13  | V     | 233 | LEU  |
| 13  | V     | 235 | ASN  |
| 13  | V     | 237 | THR  |
| 13  | V     | 239 | GLU  |
| 13  | V     | 241 | VAL  |
| 13  | V     | 244 | GLU  |
| 13  | V     | 245 | GLU  |
| 13  | V     | 249 | GLN  |
| 13  | V     | 252 | ARG  |
| 13  | V     | 255 | GLU  |
| 13  | V     | 257 | ARG  |
| 13  | V     | 259 | LYS  |
| 13  | V     | 263 | LYS  |
| 13  | V     | 265 | SER  |
| 13  | V     | 267 | ASP  |
| 13  | V     | 270 | LYS  |
| 13  | V     | 271 | LEU  |
| 13  | V     | 272 | ILE  |
| 14  | W     | 134 | VAL  |
| 14  | W     | 170 | THR  |
| 14  | W     | 171 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 85  | GLN  |
| 2   | B     | 44  | GLN  |
| 2   | B     | 92  | GLN  |
| 3   | C     | 108 | ASN  |
| 4   | D     | 25  | ASN  |
| 1   | E     | 24  | GLN  |
| 1   | E     | 68  | ASN  |
| 2   | F     | 46  | HIS  |
| 2   | F     | 92  | GLN  |
| 3   | G     | 76  | GLN  |
| 4   | H     | 75  | HIS  |
| 5   | I     | 136 | HIS  |
| 5   | I     | 204 | GLN  |
| 5   | I     | 232 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | I     | 239  | GLN  |
| 5   | I     | 702  | GLN  |
| 5   | I     | 716  | ASN  |
| 5   | I     | 719  | HIS  |
| 5   | I     | 732  | HIS  |
| 5   | I     | 780  | ASN  |
| 5   | I     | 855  | HIS  |
| 5   | I     | 892  | ASN  |
| 5   | I     | 896  | GLN  |
| 5   | I     | 902  | ASN  |
| 5   | I     | 936  | HIS  |
| 5   | I     | 1945 | HIS  |
| 5   | I     | 1963 | GLN  |
| 5   | I     | 1964 | GLN  |
| 5   | I     | 2031 | GLN  |
| 5   | I     | 2060 | HIS  |
| 6   | J     | 162  | HIS  |
| 7   | K     | 19   | HIS  |
| 7   | K     | 29   | GLN  |
| 7   | K     | 67   | ASN  |
| 7   | K     | 85   | GLN  |
| 7   | K     | 101  | ASN  |
| 7   | K     | 120  | GLN  |
| 7   | K     | 156  | HIS  |
| 7   | K     | 174  | ASN  |
| 7   | K     | 182  | ASN  |
| 7   | K     | 183  | HIS  |
| 7   | K     | 192  | GLN  |
| 7   | K     | 200  | HIS  |
| 7   | K     | 214  | GLN  |
| 7   | K     | 290  | GLN  |
| 7   | K     | 304  | ASN  |
| 7   | K     | 310  | GLN  |
| 7   | K     | 312  | HIS  |
| 7   | K     | 316  | ASN  |
| 7   | K     | 387  | HIS  |
| 8   | L     | 39   | ASN  |
| 9   | M     | 18   | HIS  |
| 9   | M     | 156  | HIS  |
| 9   | M     | 280  | ASN  |
| 10  | N     | 275  | GLN  |
| 10  | N     | 277  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | N     | 344 | HIS  |
| 10  | N     | 422 | GLN  |
| 9   | O     | 18  | HIS  |
| 9   | O     | 34  | GLN  |
| 9   | O     | 348 | HIS  |
| 9   | O     | 451 | GLN  |
| 10  | P     | 25  | HIS  |
| 10  | P     | 44  | GLN  |
| 10  | P     | 240 | HIS  |
| 10  | P     | 313 | ASN  |
| 10  | P     | 447 | GLN  |
| 9   | Q     | 18  | HIS  |
| 9   | Q     | 196 | ASN  |
| 9   | Q     | 229 | HIS  |
| 9   | Q     | 284 | ASN  |
| 9   | Q     | 373 | GLN  |
| 9   | Q     | 450 | GLN  |
| 10  | R     | 275 | GLN  |
| 10  | R     | 313 | ASN  |
| 11  | S     | 40  | HIS  |
| 11  | S     | 280 | ASN  |
| 11  | U     | 92  | ASN  |
| 11  | U     | 296 | ASN  |
| 11  | U     | 353 | GLN  |
| 13  | V     | 54  | HIS  |
| 13  | V     | 204 | ASN  |
| 13  | V     | 249 | GLN  |
| 13  | V     | 266 | GLN  |
| 13  | V     | 269 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 20  | ATP  | T     | 501  | -    | 29,33,33     | 0.28 | 0        | 44,52,52    | 0.84 | 3 (6%)   |
| 17  | ADP  | Q     | 501  | -    | 27,29,29     | 1.37 | 4 (14%)  | 42,45,45    | 1.95 | 10 (23%) |
| 17  | ADP  | N     | 501  | -    | 27,29,29     | 1.37 | 4 (14%)  | 42,45,45    | 1.91 | 11 (26%) |
| 17  | ADP  | P     | 501  | -    | 27,29,29     | 1.39 | 4 (14%)  | 42,45,45    | 2.02 | 13 (30%) |
| 17  | ADP  | R     | 501  | -    | 27,29,29     | 1.37 | 4 (14%)  | 42,45,45    | 1.95 | 10 (23%) |
| 19  | BEF  | I     | 3303 | -    | 0,3,3        | -    | -        | -           | -    | -        |
| 20  | ATP  | U     | 401  | -    | 29,33,33     | 0.30 | 0        | 44,52,52    | 0.79 | 1 (2%)   |
| 17  | ADP  | M     | 501  | -    | 27,29,29     | 1.35 | 4 (14%)  | 42,45,45    | 2.01 | 8 (19%)  |
| 17  | ADP  | O     | 501  | -    | 27,29,29     | 1.40 | 4 (14%)  | 42,45,45    | 1.96 | 10 (23%) |
| 17  | ADP  | I     | 3301 | -    | 27,29,29     | 1.36 | 5 (18%)  | 42,45,45    | 1.99 | 12 (28%) |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 20  | ATP  | T     | 501  | -    | -       | 1/22/38/38 | 0/3/3/3 |
| 17  | ADP  | Q     | 501  | -    | -       | 3/16/32/32 | 0/3/3/3 |
| 17  | ADP  | N     | 501  | -    | -       | 4/16/32/32 | 0/3/3/3 |
| 17  | ADP  | P     | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 17  | ADP  | R     | 501  | -    | -       | 1/16/32/32 | 0/3/3/3 |
| 20  | ATP  | U     | 401  | -    | -       | 2/22/38/38 | 0/3/3/3 |
| 17  | ADP  | M     | 501  | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 17  | ADP  | O     | 501  | -    | -       | 6/16/32/32 | 0/3/3/3 |
| 17  | ADP  | I     | 3301 | -    | -       | 5/16/32/32 | 0/3/3/3 |

All (29) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 17  | O     | 501  | ADP  | C5-C4 | 4.81  | 1.48        | 1.39     |
| 17  | R     | 501  | ADP  | C5-C4 | 4.71  | 1.47        | 1.39     |
| 17  | P     | 501  | ADP  | C5-C4 | 4.71  | 1.47        | 1.39     |
| 17  | Q     | 501  | ADP  | C5-C4 | 4.70  | 1.47        | 1.39     |
| 17  | M     | 501  | ADP  | C5-C4 | 4.68  | 1.47        | 1.39     |
| 17  | N     | 501  | ADP  | C5-C4 | 4.56  | 1.47        | 1.39     |
| 17  | I     | 3301 | ADP  | C5-C4 | 4.56  | 1.47        | 1.39     |
| 17  | P     | 501  | ADP  | C5-C6 | 2.79  | 1.48        | 1.41     |
| 17  | O     | 501  | ADP  | C5-C6 | 2.72  | 1.48        | 1.41     |
| 17  | N     | 501  | ADP  | C5-C6 | 2.69  | 1.48        | 1.41     |
| 17  | Q     | 501  | ADP  | C5-C6 | 2.69  | 1.48        | 1.41     |
| 17  | R     | 501  | ADP  | C5-C6 | 2.67  | 1.48        | 1.41     |
| 17  | M     | 501  | ADP  | C5-C6 | 2.53  | 1.48        | 1.41     |
| 17  | I     | 3301 | ADP  | C5-C6 | 2.51  | 1.48        | 1.41     |
| 17  | O     | 501  | ADP  | C5-N7 | -2.42 | 1.34        | 1.39     |
| 17  | I     | 3301 | ADP  | C8-N7 | 2.37  | 1.36        | 1.31     |
| 17  | M     | 501  | ADP  | C5-N7 | -2.36 | 1.34        | 1.39     |
| 17  | P     | 501  | ADP  | C5-N7 | -2.32 | 1.34        | 1.39     |
| 17  | P     | 501  | ADP  | C8-N7 | 2.30  | 1.36        | 1.31     |
| 17  | N     | 501  | ADP  | C8-N7 | 2.29  | 1.35        | 1.31     |
| 17  | Q     | 501  | ADP  | C5-N7 | -2.28 | 1.34        | 1.39     |
| 17  | N     | 501  | ADP  | C5-N7 | -2.27 | 1.34        | 1.39     |
| 17  | R     | 501  | ADP  | C5-N7 | -2.26 | 1.34        | 1.39     |
| 17  | O     | 501  | ADP  | C8-N7 | 2.24  | 1.35        | 1.31     |
| 17  | Q     | 501  | ADP  | C8-N7 | 2.24  | 1.35        | 1.31     |
| 17  | I     | 3301 | ADP  | C5-N7 | -2.20 | 1.34        | 1.39     |
| 17  | R     | 501  | ADP  | C8-N7 | 2.14  | 1.35        | 1.31     |
| 17  | I     | 3301 | ADP  | C4-N9 | -2.05 | 1.33        | 1.37     |
| 17  | M     | 501  | ADP  | C8-N7 | 2.04  | 1.35        | 1.31     |

All (78) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 17  | M     | 501  | ADP  | C5-C4-N3 | -6.38 | 118.43      | 126.75   |
| 17  | P     | 501  | ADP  | C5-C4-N3 | -6.34 | 118.48      | 126.75   |
| 17  | O     | 501  | ADP  | C5-C4-N3 | -6.22 | 118.64      | 126.75   |
| 17  | R     | 501  | ADP  | C5-C4-N3 | -6.20 | 118.66      | 126.75   |
| 17  | N     | 501  | ADP  | C5-C4-N3 | -6.06 | 118.84      | 126.75   |
| 17  | Q     | 501  | ADP  | C5-C4-N3 | -6.05 | 118.86      | 126.75   |
| 17  | I     | 3301 | ADP  | C5-C4-N3 | -5.36 | 119.75      | 126.75   |
| 17  | M     | 501  | ADP  | N3-C4-N9 | 5.22  | 135.68      | 127.08   |
| 17  | R     | 501  | ADP  | N3-C4-N9 | 4.92  | 135.20      | 127.08   |
| 17  | P     | 501  | ADP  | N3-C4-N9 | 4.91  | 135.18      | 127.08   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | O     | 501  | ADP  | N3-C4-N9    | 4.82  | 135.02      | 127.08   |
| 17  | Q     | 501  | ADP  | N3-C4-N9    | 4.81  | 135.00      | 127.08   |
| 17  | N     | 501  | ADP  | N3-C4-N9    | 4.67  | 134.78      | 127.08   |
| 17  | I     | 3301 | ADP  | N3-C4-N9    | 4.46  | 134.43      | 127.08   |
| 17  | I     | 3301 | ADP  | PA-O3A-PB   | -4.37 | 117.84      | 132.83   |
| 17  | P     | 501  | ADP  | C2-N3-C4    | 3.87  | 120.89      | 111.75   |
| 17  | M     | 501  | ADP  | C2-N3-C4    | 3.87  | 120.88      | 111.75   |
| 17  | N     | 501  | ADP  | C2-N3-C4    | 3.86  | 120.86      | 111.75   |
| 17  | O     | 501  | ADP  | C2-N3-C4    | 3.85  | 120.83      | 111.75   |
| 17  | R     | 501  | ADP  | C2-N3-C4    | 3.83  | 120.79      | 111.75   |
| 17  | Q     | 501  | ADP  | C2-N3-C4    | 3.75  | 120.62      | 111.75   |
| 17  | I     | 3301 | ADP  | C2-N3-C4    | 3.67  | 120.43      | 111.75   |
| 17  | Q     | 501  | ADP  | PA-O3A-PB   | -3.64 | 120.34      | 132.83   |
| 17  | M     | 501  | ADP  | PA-O3A-PB   | -3.51 | 120.79      | 132.83   |
| 17  | N     | 501  | ADP  | C4-C5-N7    | -3.49 | 106.37      | 110.62   |
| 17  | P     | 501  | ADP  | C4-C5-N7    | -3.48 | 106.38      | 110.62   |
| 17  | I     | 3301 | ADP  | N3-C2-N1    | -3.48 | 123.16      | 128.60   |
| 17  | O     | 501  | ADP  | C4-C5-N7    | -3.40 | 106.48      | 110.62   |
| 17  | R     | 501  | ADP  | PA-O3A-PB   | -3.40 | 121.17      | 132.83   |
| 17  | O     | 501  | ADP  | PA-O3A-PB   | -3.39 | 121.19      | 132.83   |
| 17  | R     | 501  | ADP  | C4-C5-N7    | -3.36 | 106.53      | 110.62   |
| 17  | O     | 501  | ADP  | N3-C2-N1    | -3.33 | 123.40      | 128.60   |
| 17  | Q     | 501  | ADP  | C4-C5-N7    | -3.32 | 106.57      | 110.62   |
| 17  | N     | 501  | ADP  | N3-C2-N1    | -3.31 | 123.43      | 128.60   |
| 17  | Q     | 501  | ADP  | N3-C2-N1    | -3.30 | 123.44      | 128.60   |
| 17  | R     | 501  | ADP  | N3-C2-N1    | -3.26 | 123.50      | 128.60   |
| 17  | M     | 501  | ADP  | N3-C2-N1    | -3.25 | 123.52      | 128.60   |
| 17  | N     | 501  | ADP  | PA-O3A-PB   | -3.21 | 121.83      | 132.83   |
| 17  | P     | 501  | ADP  | N3-C2-N1    | -3.19 | 123.62      | 128.60   |
| 17  | P     | 501  | ADP  | PA-O3A-PB   | -3.18 | 121.93      | 132.83   |
| 17  | M     | 501  | ADP  | C4-C5-N7    | -3.15 | 106.78      | 110.62   |
| 17  | P     | 501  | ADP  | C5-N7-C8    | 3.01  | 107.79      | 103.51   |
| 17  | N     | 501  | ADP  | C5-N7-C8    | 2.98  | 107.74      | 103.51   |
| 17  | I     | 3301 | ADP  | C4-N9-C8    | 2.97  | 108.94      | 105.73   |
| 17  | R     | 501  | ADP  | C5-N7-C8    | 2.89  | 107.61      | 103.51   |
| 17  | O     | 501  | ADP  | C5-N7-C8    | 2.89  | 107.61      | 103.51   |
| 17  | Q     | 501  | ADP  | C5-N7-C8    | 2.87  | 107.59      | 103.51   |
| 17  | M     | 501  | ADP  | C5-N7-C8    | 2.87  | 107.58      | 103.51   |
| 17  | I     | 3301 | ADP  | C4-C5-N7    | -2.85 | 107.15      | 110.62   |
| 17  | P     | 501  | ADP  | C3'-C2'-C1' | 2.72  | 106.60      | 101.43   |
| 17  | I     | 3301 | ADP  | C2'-C1'-N9  | -2.72 | 106.41      | 113.30   |
| 17  | N     | 501  | ADP  | C4-N9-C8    | 2.65  | 108.60      | 105.73   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | Q     | 501  | ADP  | C4-N9-C8    | 2.56  | 108.50      | 105.73   |
| 17  | R     | 501  | ADP  | C4-N9-C8    | 2.53  | 108.47      | 105.73   |
| 17  | M     | 501  | ADP  | C4-N9-C8    | 2.50  | 108.44      | 105.73   |
| 17  | I     | 3301 | ADP  | C3'-C2'-C1' | 2.45  | 106.09      | 101.43   |
| 17  | N     | 501  | ADP  | C6-C5-N7    | 2.41  | 136.51      | 132.02   |
| 17  | P     | 501  | ADP  | C4-N9-C8    | 2.41  | 108.34      | 105.73   |
| 17  | I     | 3301 | ADP  | C6-C5-N7    | 2.39  | 136.48      | 132.02   |
| 17  | I     | 3301 | ADP  | C5-N7-C8    | 2.34  | 106.83      | 103.51   |
| 17  | Q     | 501  | ADP  | C2-N1-C6    | 2.31  | 122.73      | 118.77   |
| 17  | O     | 501  | ADP  | C2-N1-C6    | 2.25  | 122.62      | 118.77   |
| 17  | O     | 501  | ADP  | C4-N9-C8    | 2.23  | 108.14      | 105.73   |
| 17  | R     | 501  | ADP  | C6-C5-N7    | 2.22  | 136.15      | 132.02   |
| 17  | P     | 501  | ADP  | C6-C5-N7    | 2.22  | 136.15      | 132.02   |
| 17  | N     | 501  | ADP  | N9-C8-N7    | -2.20 | 110.91      | 113.91   |
| 20  | T     | 501  | ATP  | O3'-C3'-C2' | -2.19 | 104.72      | 111.82   |
| 20  | U     | 401  | ATP  | O3'-C3'-C2' | -2.18 | 104.77      | 111.82   |
| 20  | T     | 501  | ATP  | O3'-C3'-C4' | -2.17 | 104.77      | 111.05   |
| 17  | Q     | 501  | ADP  | C6-C5-N7    | 2.15  | 136.03      | 132.02   |
| 17  | O     | 501  | ADP  | C6-C5-N7    | 2.15  | 136.03      | 132.02   |
| 17  | I     | 3301 | ADP  | C2-N1-C6    | 2.14  | 122.45      | 118.77   |
| 17  | R     | 501  | ADP  | C2-N1-C6    | 2.07  | 122.32      | 118.77   |
| 20  | T     | 501  | ATP  | PB-O3B-PG   | 2.07  | 139.92      | 132.83   |
| 17  | P     | 501  | ADP  | O3B-PB-O2B  | 2.03  | 115.41      | 107.64   |
| 17  | P     | 501  | ADP  | C2-N1-C6    | 2.03  | 122.25      | 118.77   |
| 17  | N     | 501  | ADP  | C2-N1-C6    | 2.02  | 122.23      | 118.77   |
| 17  | P     | 501  | ADP  | N9-C8-N7    | -2.02 | 111.15      | 113.91   |

There are no chirality outliers.

All (26) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | I     | 3301 | ADP  | C5'-O5'-PA-O2A  |
| 17  | N     | 501  | ADP  | C5'-O5'-PA-O1A  |
| 17  | N     | 501  | ADP  | O4'-C4'-C5'-O5' |
| 17  | O     | 501  | ADP  | C5'-O5'-PA-O2A  |
| 17  | P     | 501  | ADP  | PA-O3A-PB-O2B   |
| 17  | N     | 501  | ADP  | C3'-C4'-C5'-O5' |
| 20  | U     | 401  | ATP  | C3'-C4'-C5'-O5' |
| 17  | I     | 3301 | ADP  | O4'-C4'-C5'-O5' |
| 17  | I     | 3301 | ADP  | C3'-C4'-C5'-O5' |
| 17  | O     | 501  | ADP  | O4'-C4'-C5'-O5' |
| 17  | M     | 501  | ADP  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | I     | 3301 | ADP  | C5'-O5'-PA-O3A  |
| 17  | O     | 501  | ADP  | C5'-O5'-PA-O3A  |
| 17  | O     | 501  | ADP  | C3'-C4'-C5'-O5' |
| 17  | Q     | 501  | ADP  | O4'-C4'-C5'-O5' |
| 17  | I     | 3301 | ADP  | C5'-O5'-PA-O1A  |
| 17  | O     | 501  | ADP  | C4'-C5'-O5'-PA  |
| 20  | U     | 401  | ATP  | O4'-C4'-C5'-O5' |
| 17  | Q     | 501  | ADP  | C4'-C5'-O5'-PA  |
| 17  | Q     | 501  | ADP  | C3'-C4'-C5'-O5' |
| 17  | P     | 501  | ADP  | PA-O3A-PB-O3B   |
| 17  | M     | 501  | ADP  | C5'-O5'-PA-O3A  |
| 17  | N     | 501  | ADP  | C5'-O5'-PA-O3A  |
| 20  | T     | 501  | ATP  | C3'-C4'-C5'-O5' |
| 17  | R     | 501  | ADP  | C4'-C5'-O5'-PA  |
| 17  | O     | 501  | ADP  | C5'-O5'-PA-O1A  |

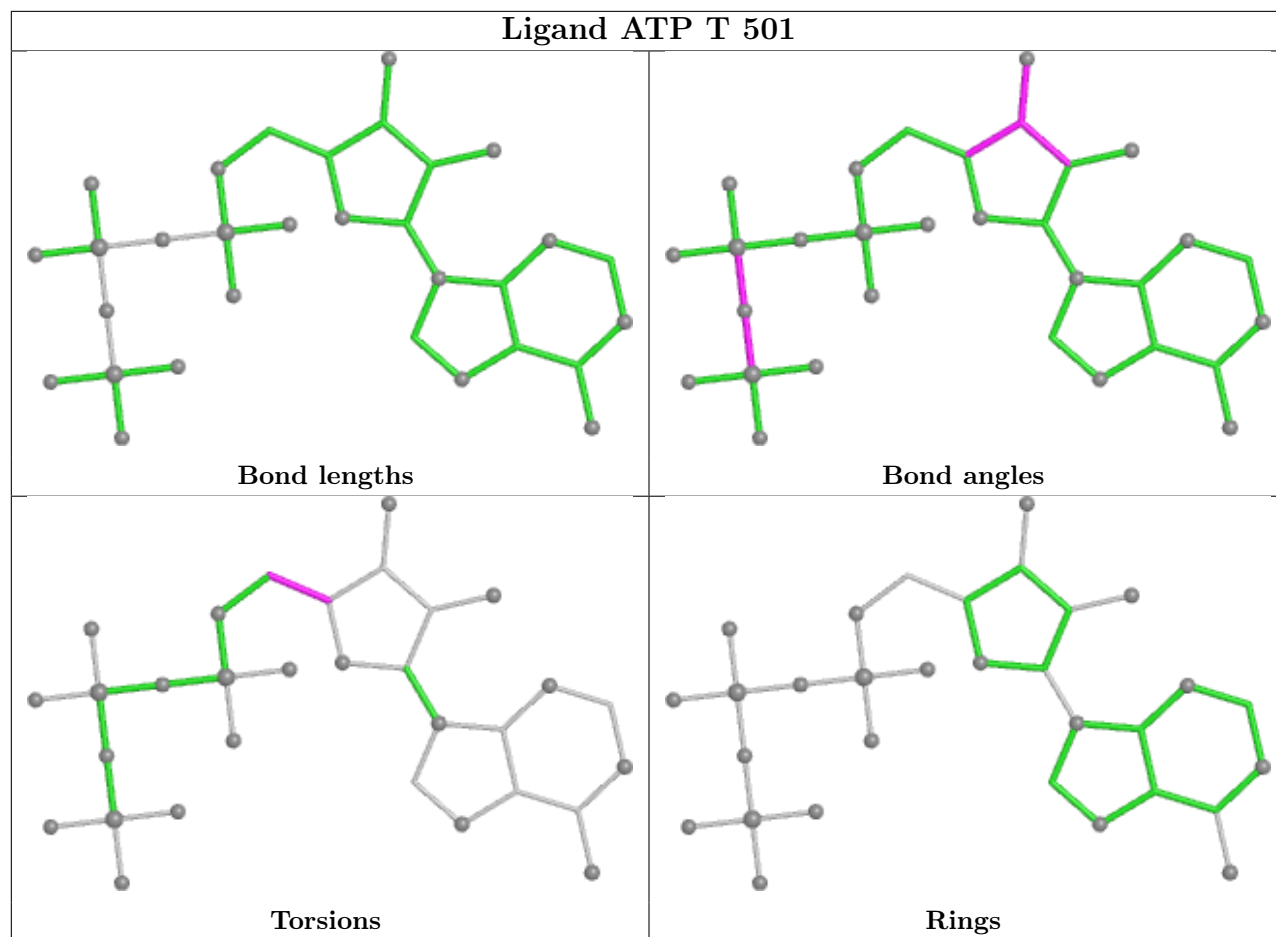
There are no ring outliers.

4 monomers are involved in 10 short contacts:

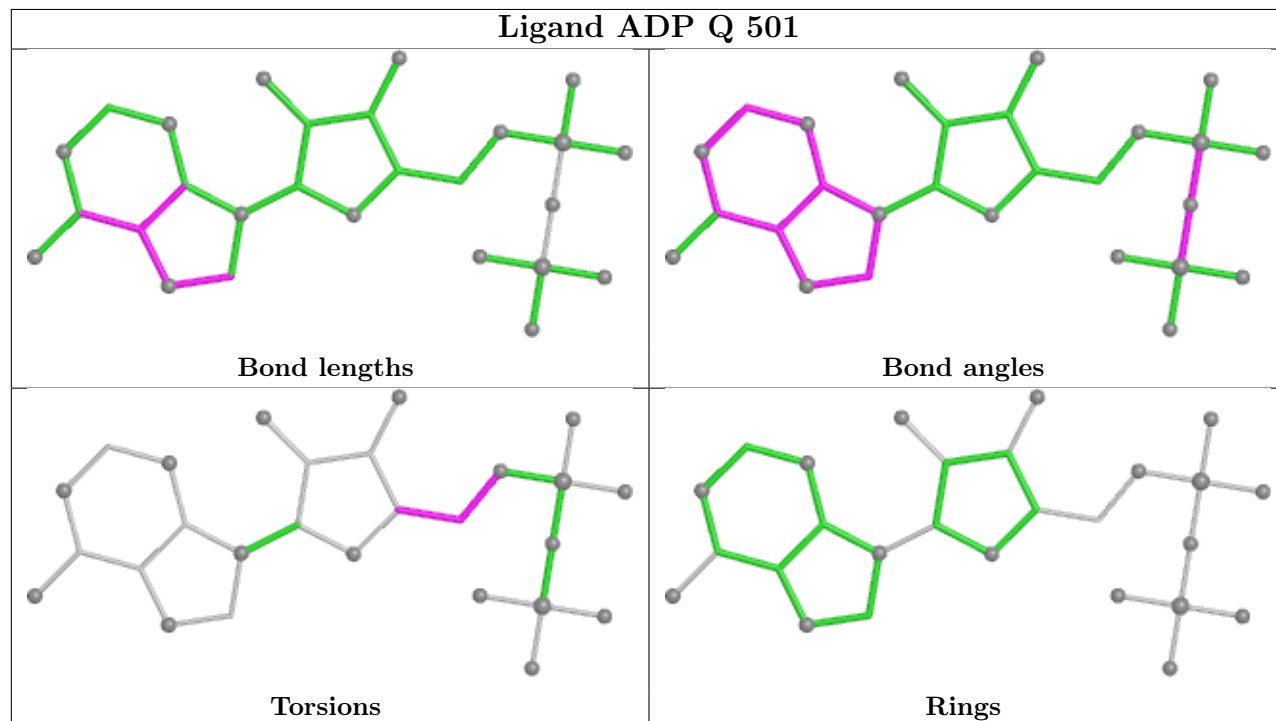
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 20  | T     | 501  | ATP  | 1       | 0            |
| 19  | I     | 3303 | BEF  | 3       | 0            |
| 17  | O     | 501  | ADP  | 1       | 0            |
| 17  | I     | 3301 | ADP  | 6       | 0            |

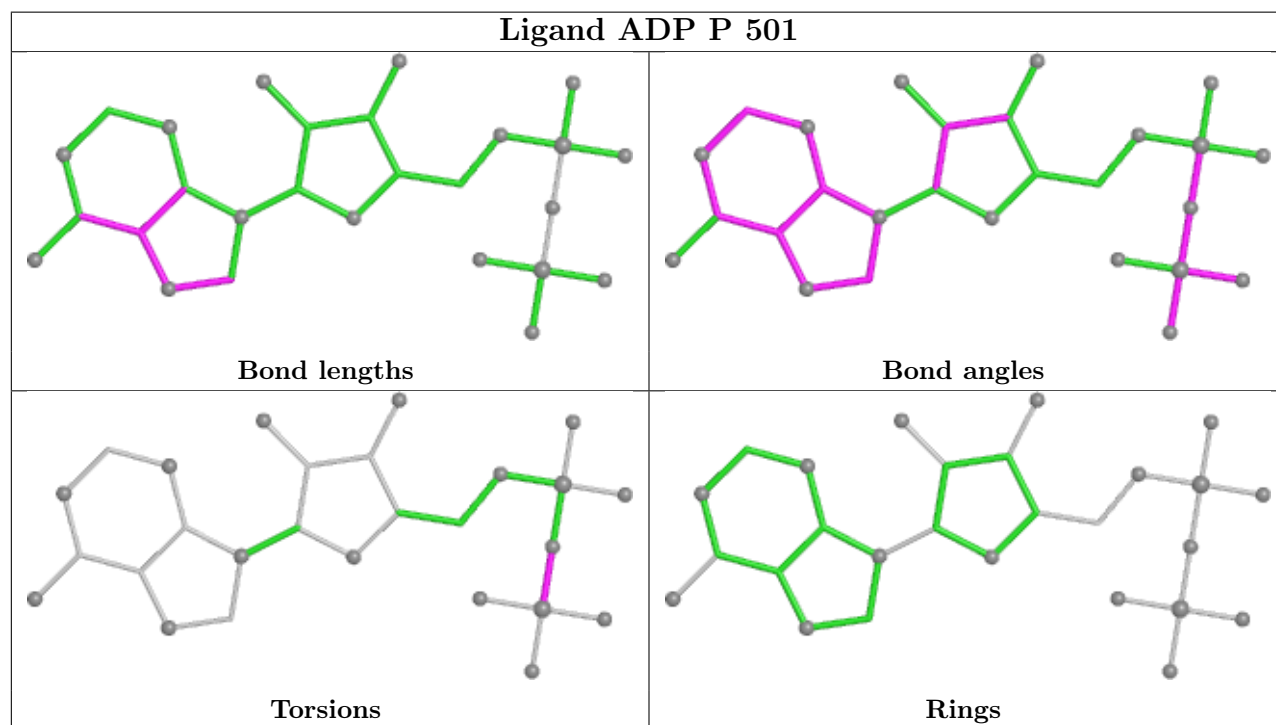
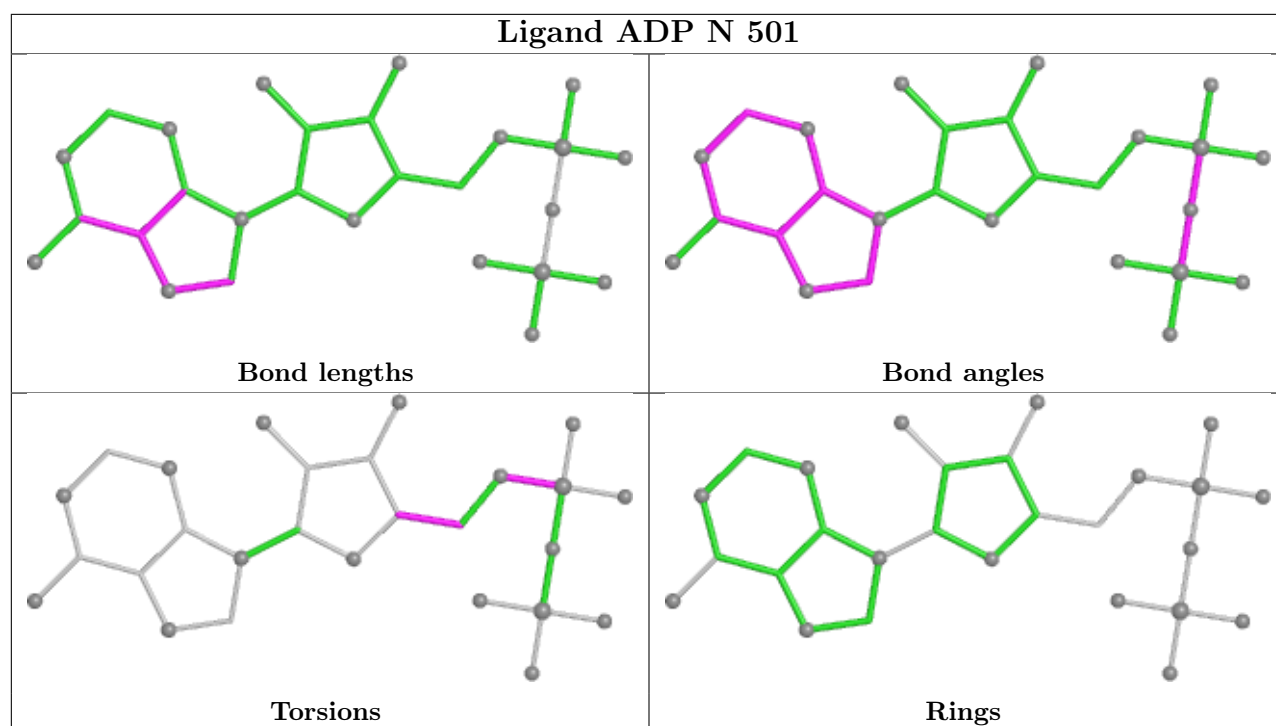
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

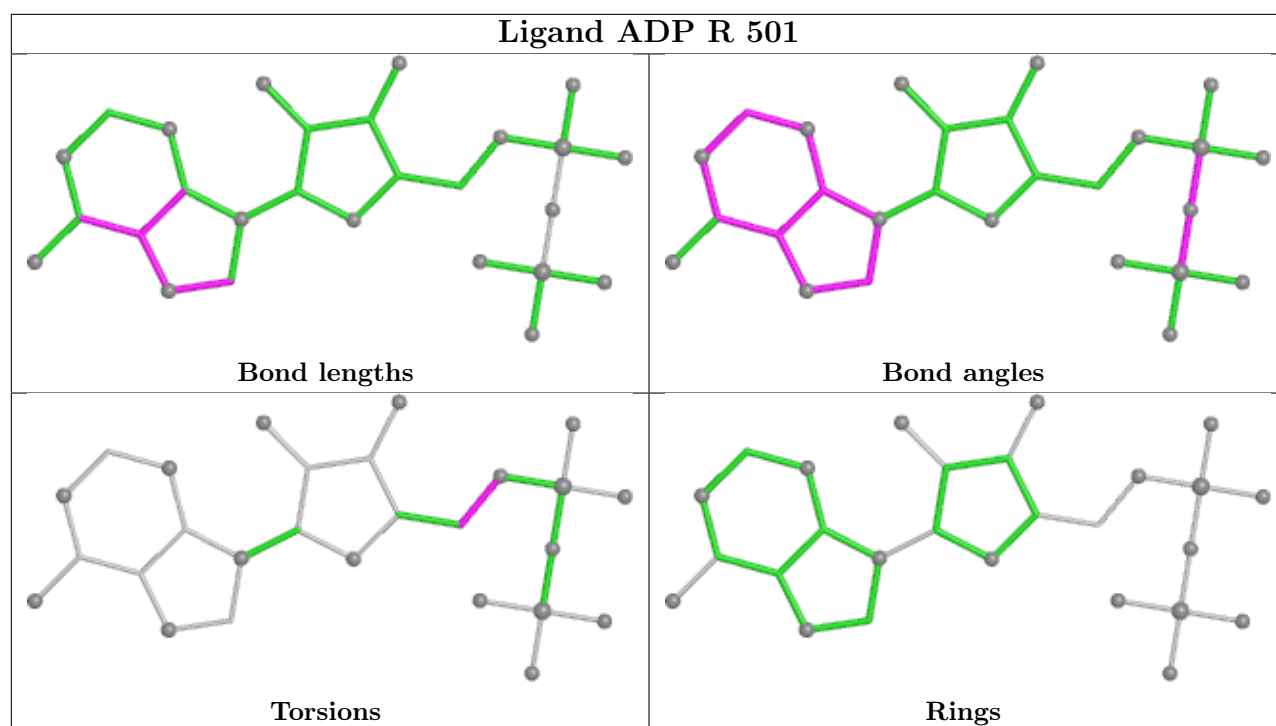
## Ligand ATP T 501

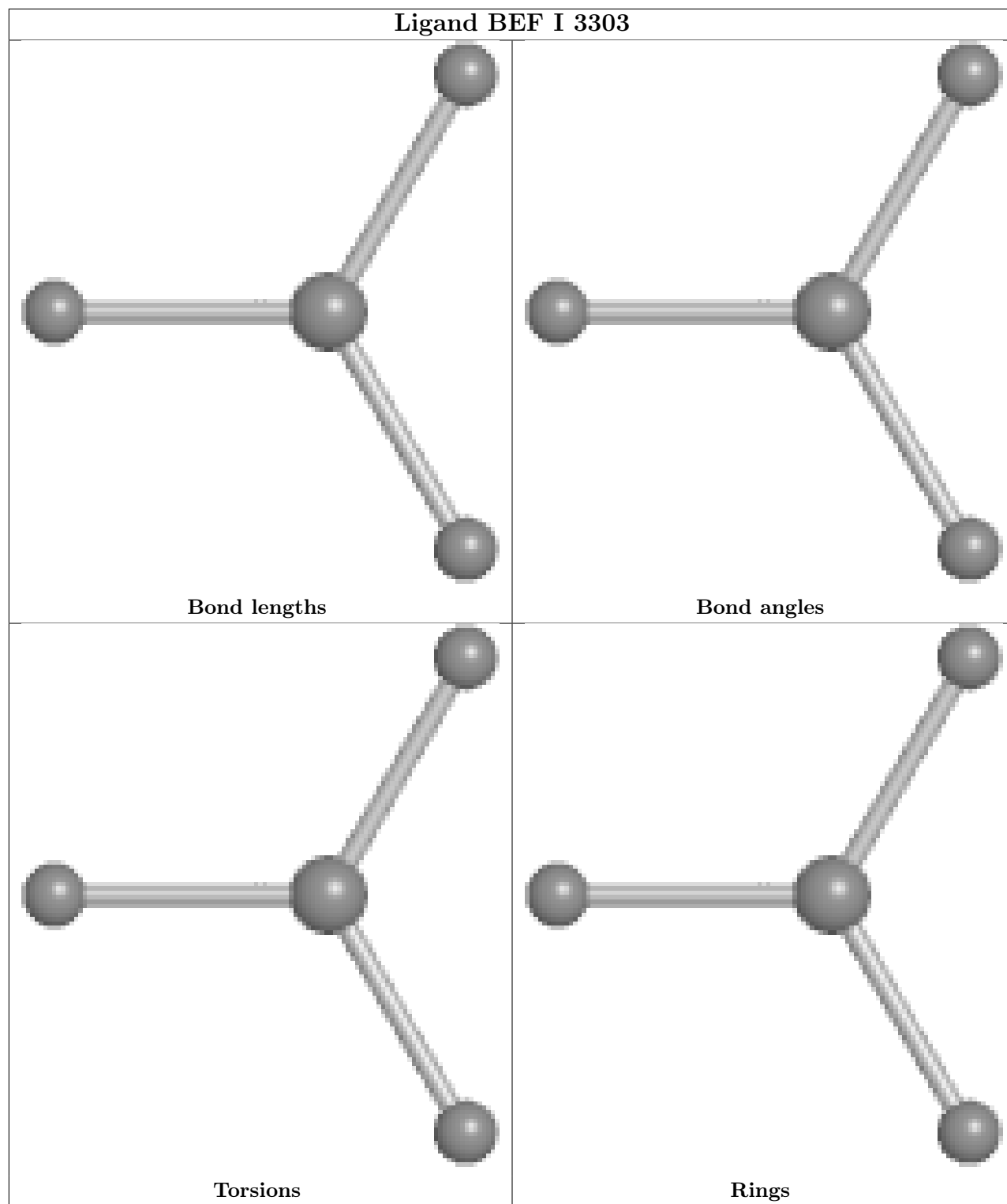


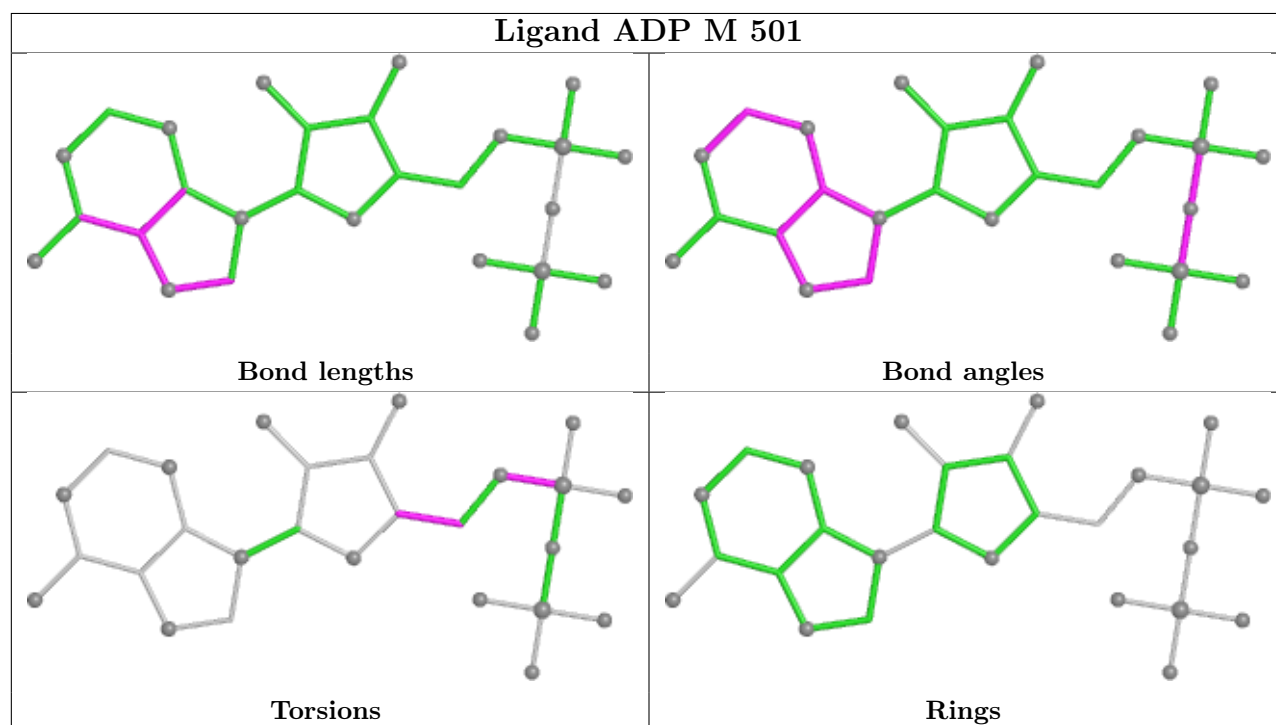
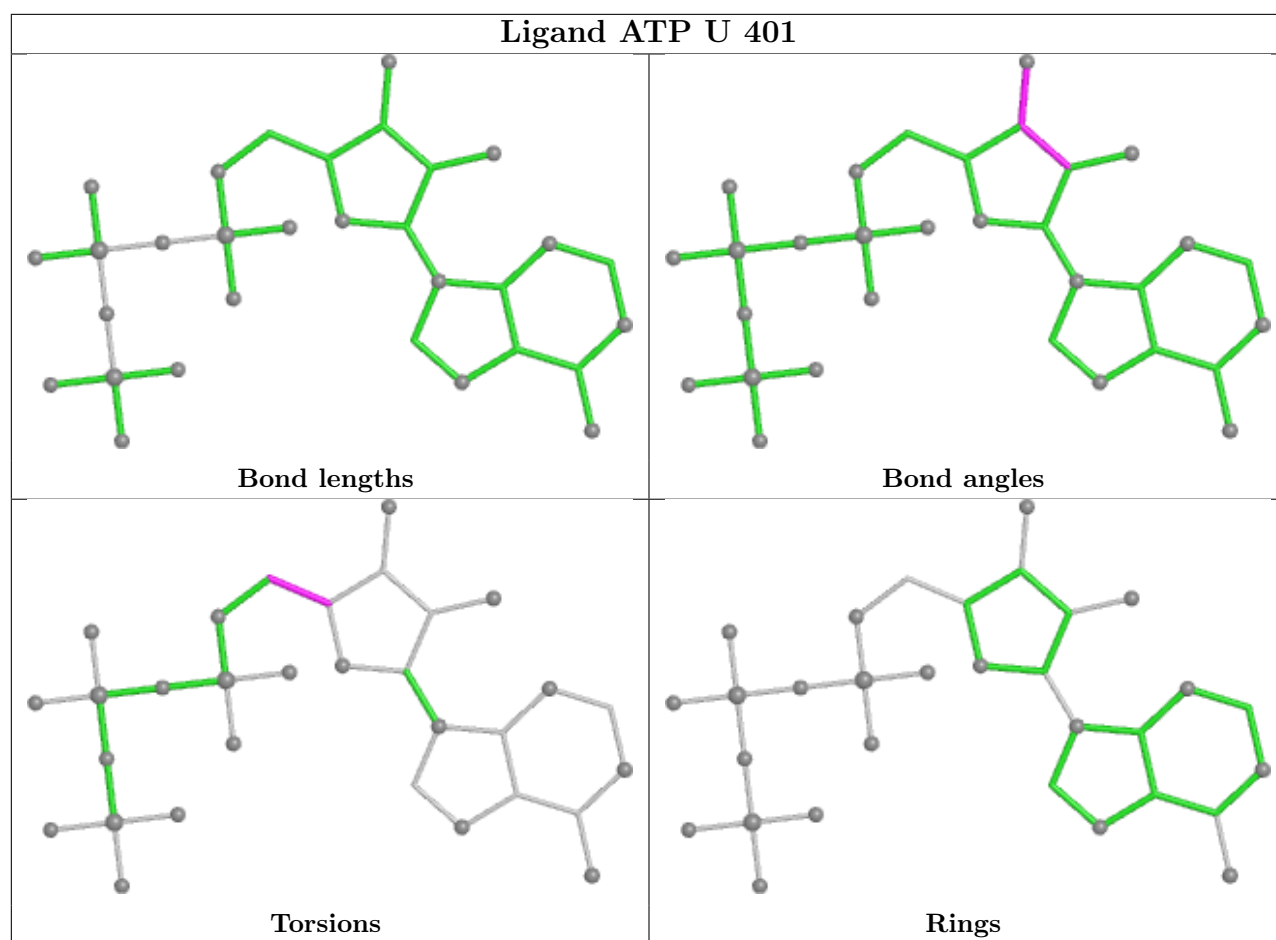
## Ligand ADP Q 501

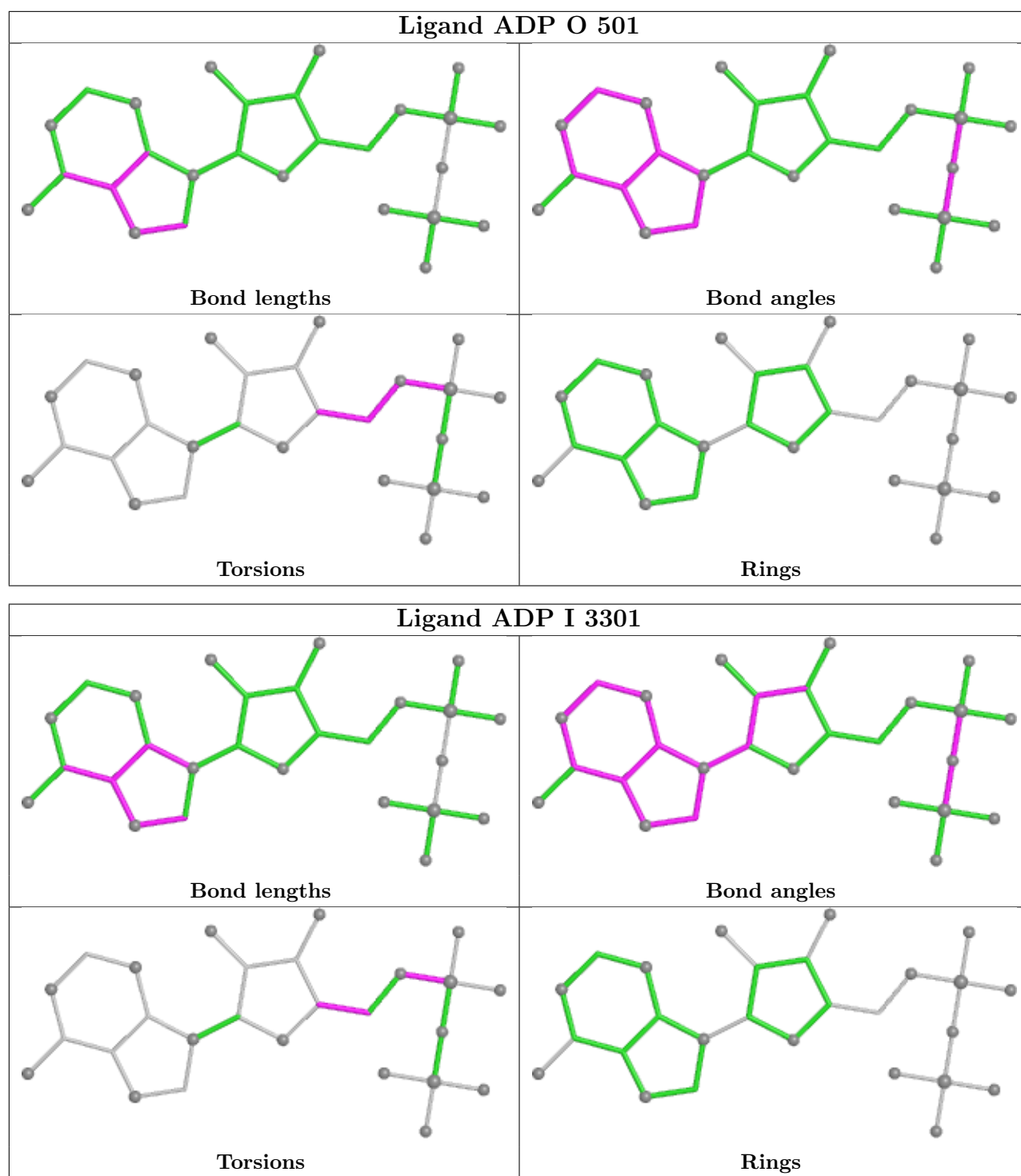












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

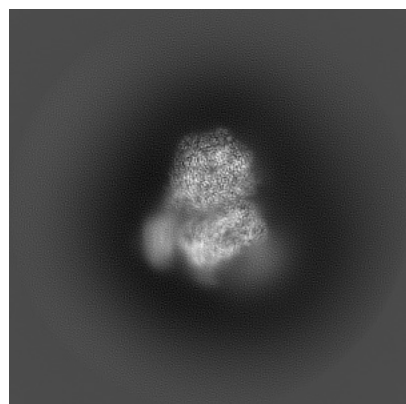
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37988. These allow visual inspection of the internal detail of the map and identification of artifacts.

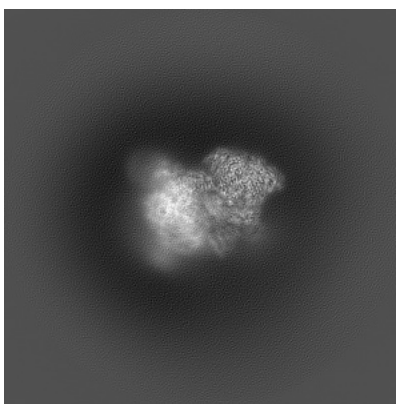
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

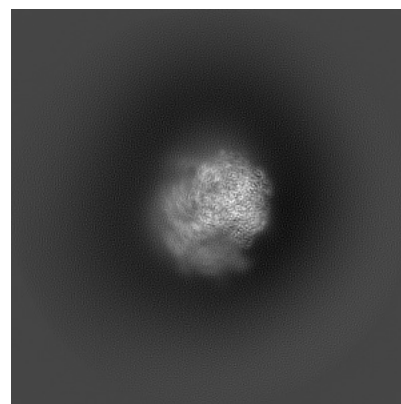
#### 6.1.1 Primary map



X

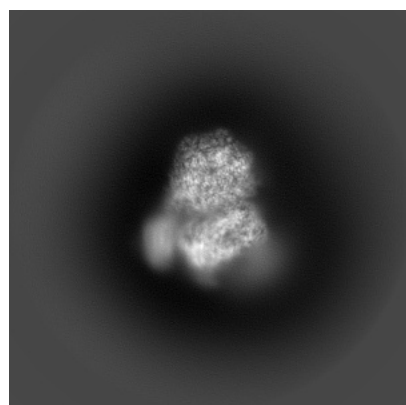


Y

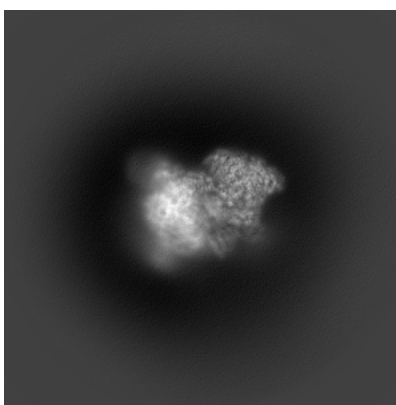


Z

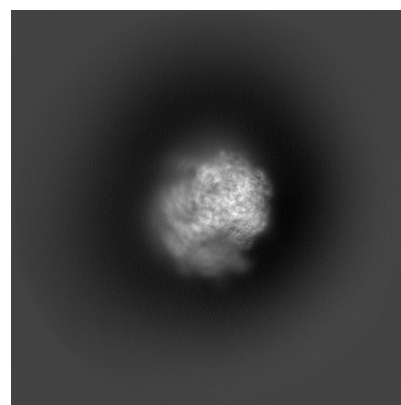
#### 6.1.2 Raw map



X



Y

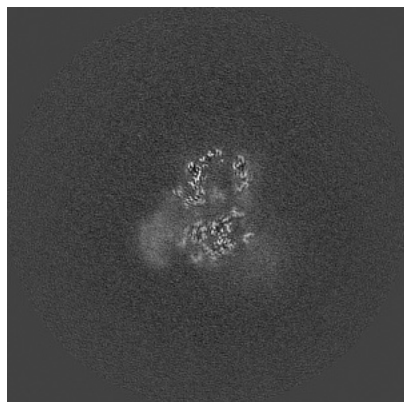


Z

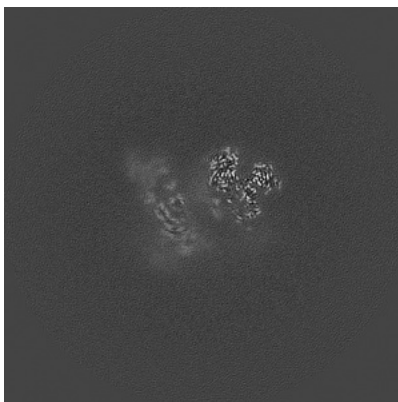
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

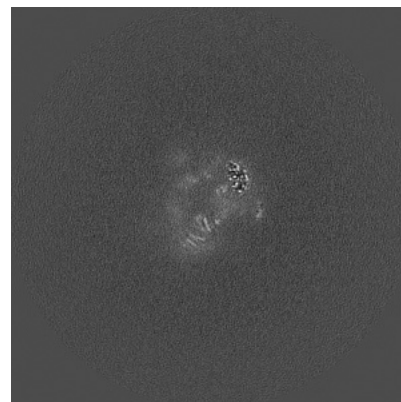
### 6.2.1 Primary map



X Index: 200

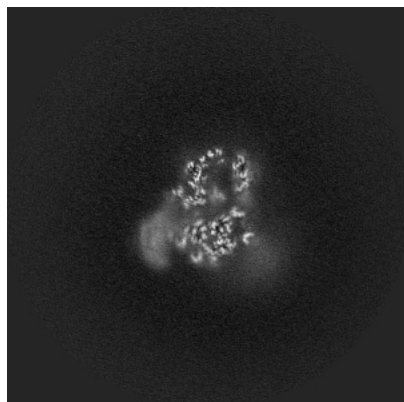


Y Index: 200

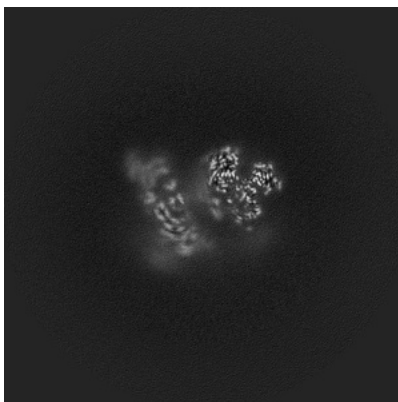


Z Index: 200

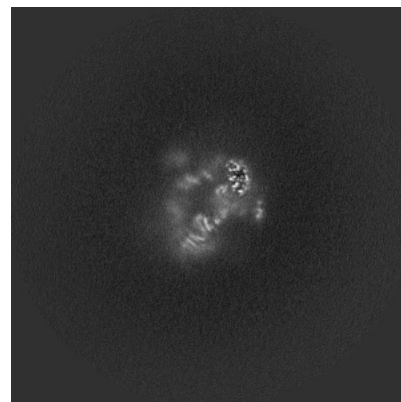
### 6.2.2 Raw map



X Index: 200



Y Index: 200

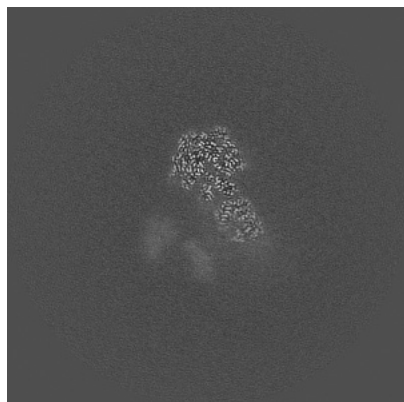


Z Index: 200

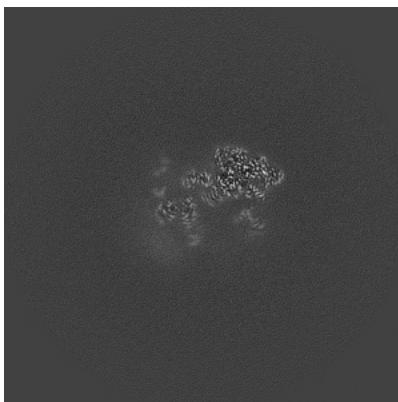
The images above show central slices of the map in three orthogonal directions.

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

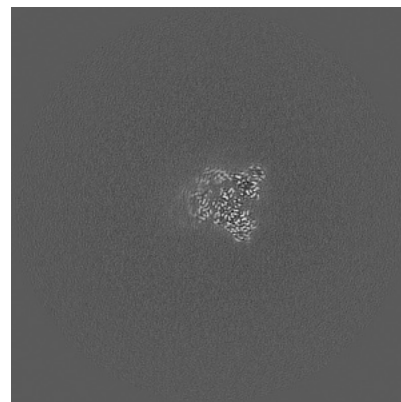
### 6.3.1 Primary map



X Index: 228

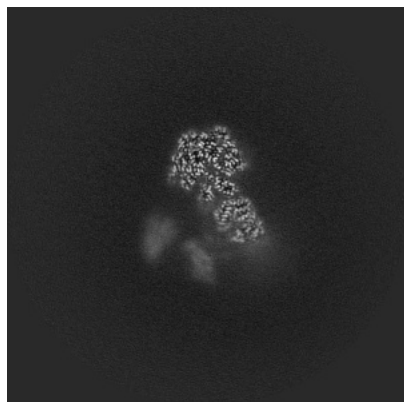


Y Index: 217

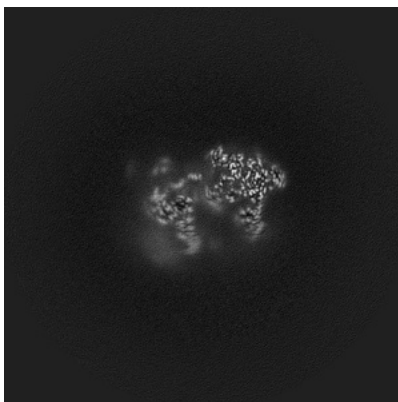


Z Index: 246

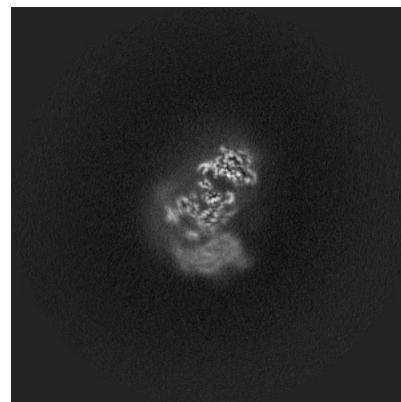
### 6.3.2 Raw map



X Index: 228



Y Index: 210

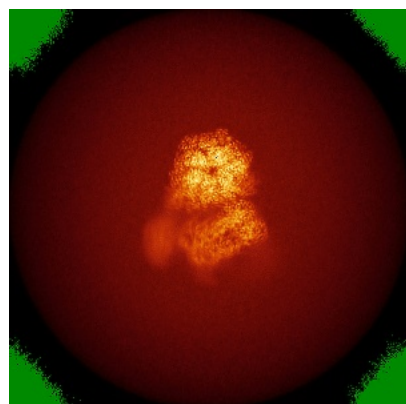


Z Index: 173

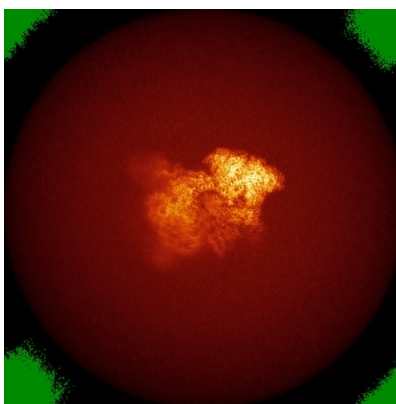
The images above show the largest variance slices of the map in three orthogonal directions.

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

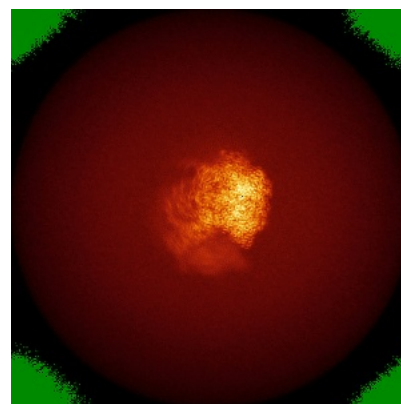
### 6.4.1 Primary map



X

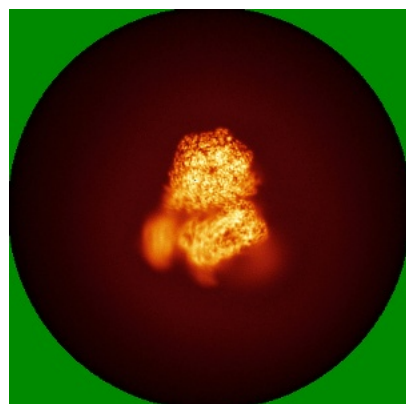


Y

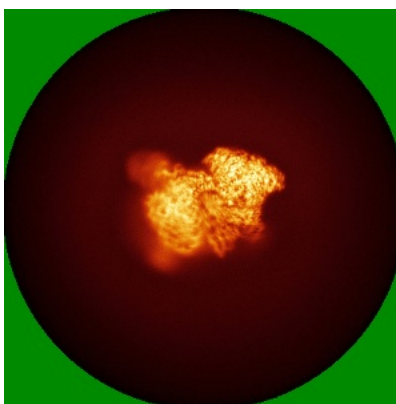


Z

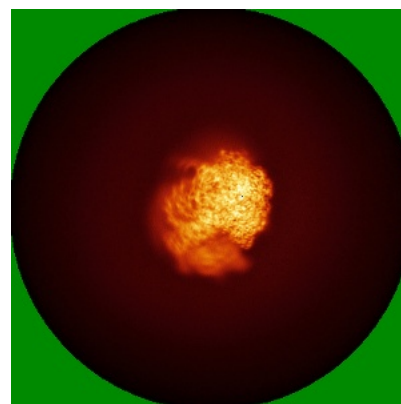
### 6.4.2 Raw map



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



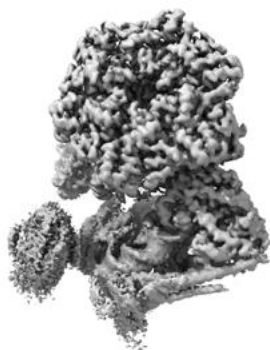
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

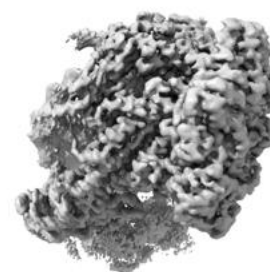
### 6.5.2 Raw map



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.

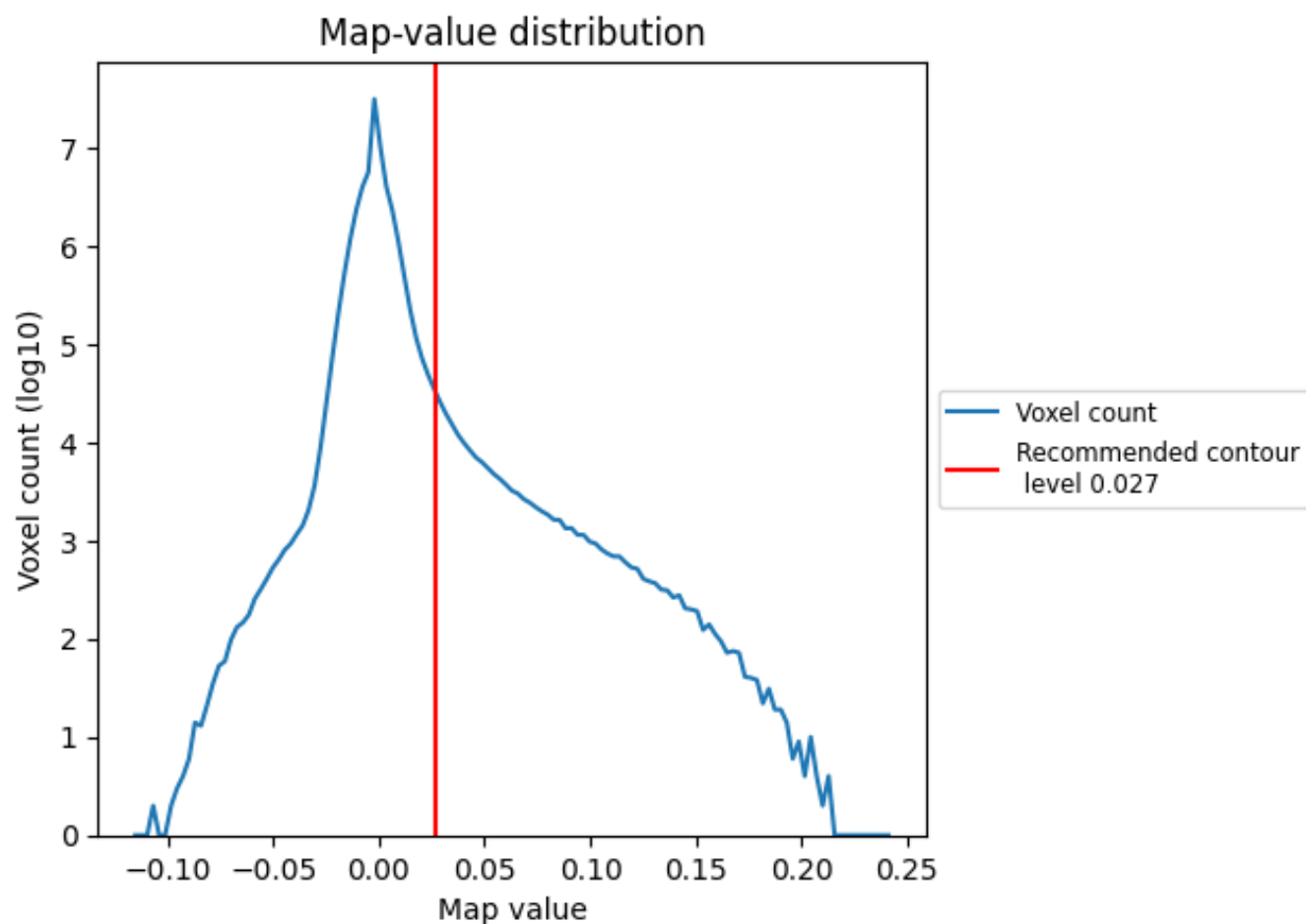
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

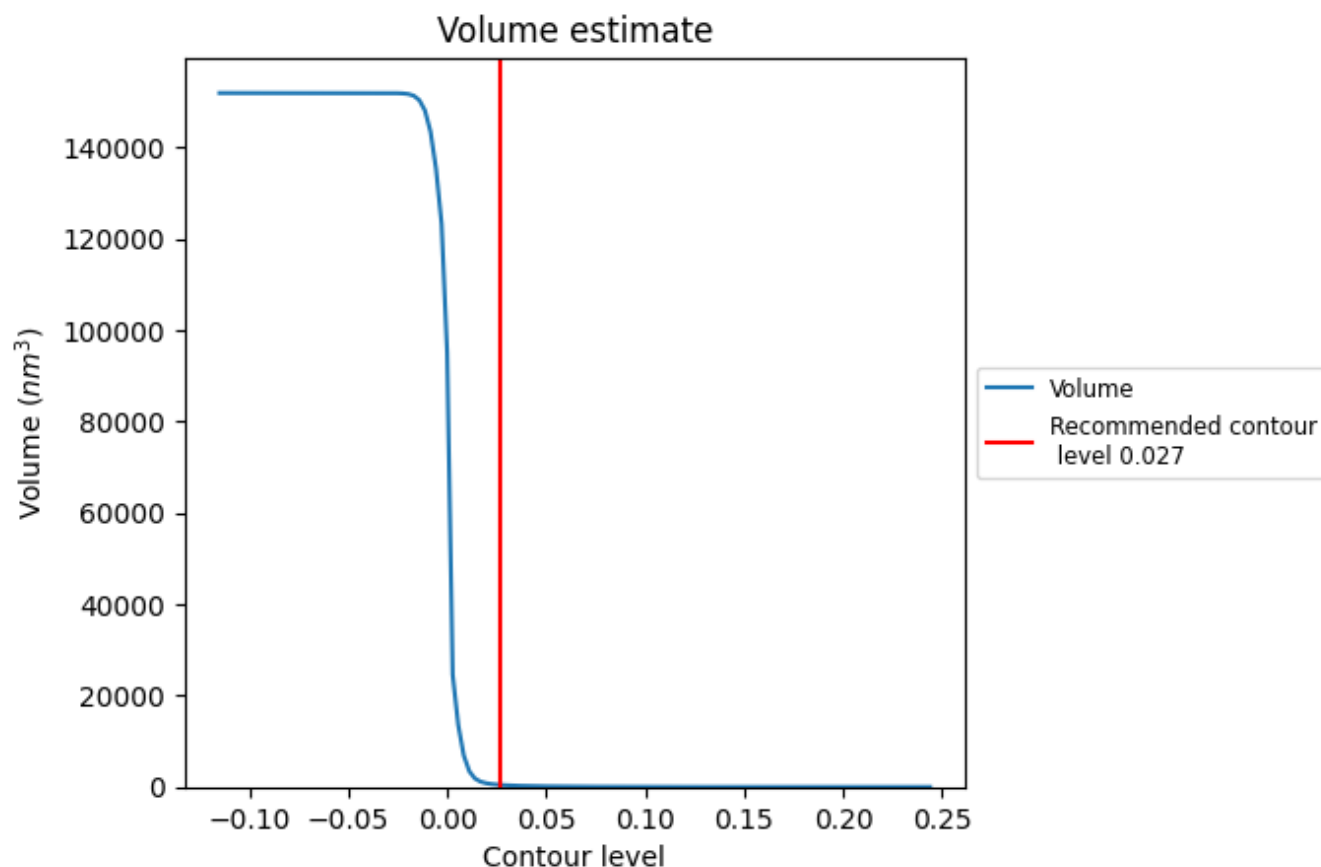
This section contains the results of statistical analysis of the map.

### 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.

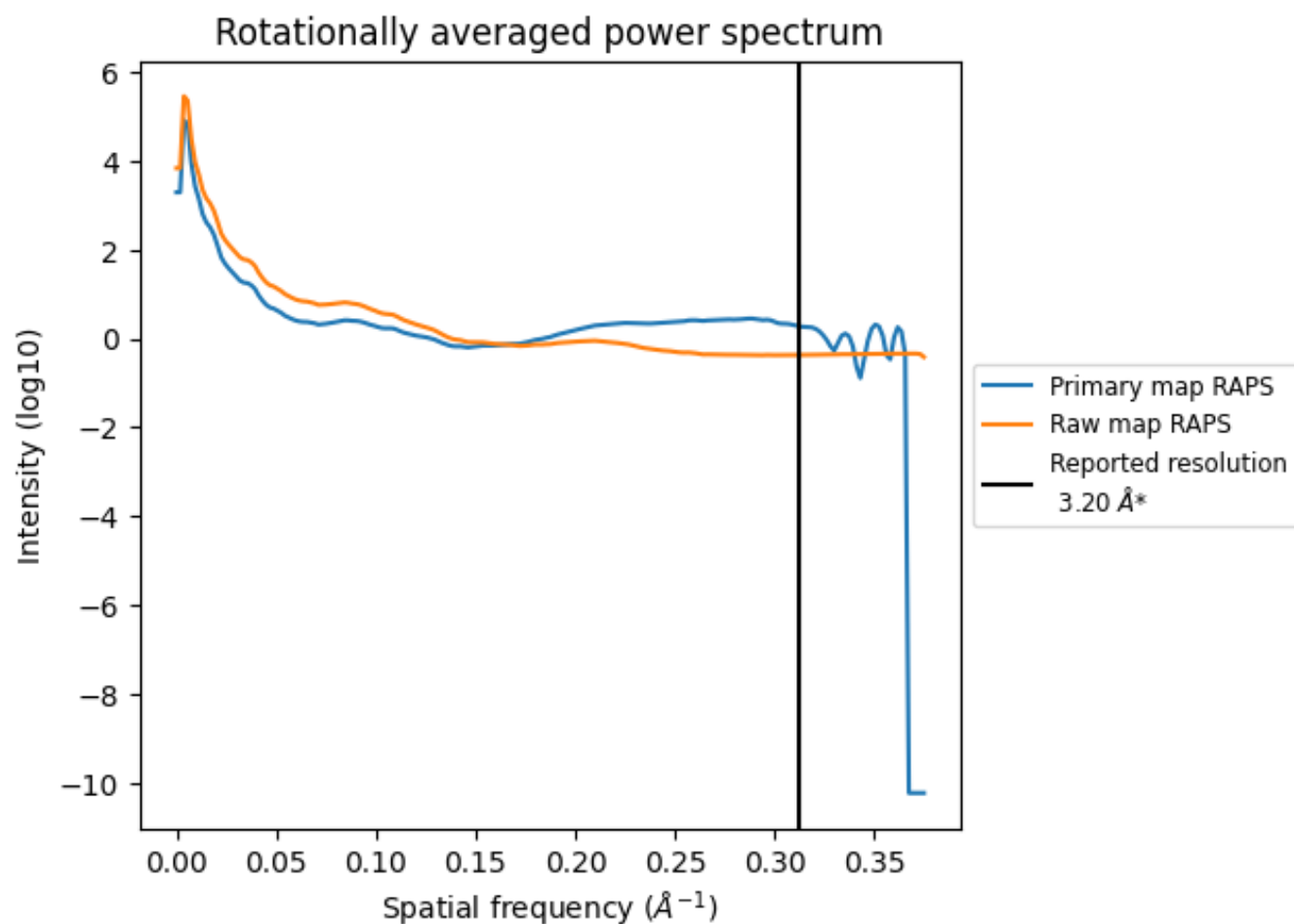
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 435  $\text{nm}^3$ ; this corresponds to an approximate mass of 393 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 ⓘ

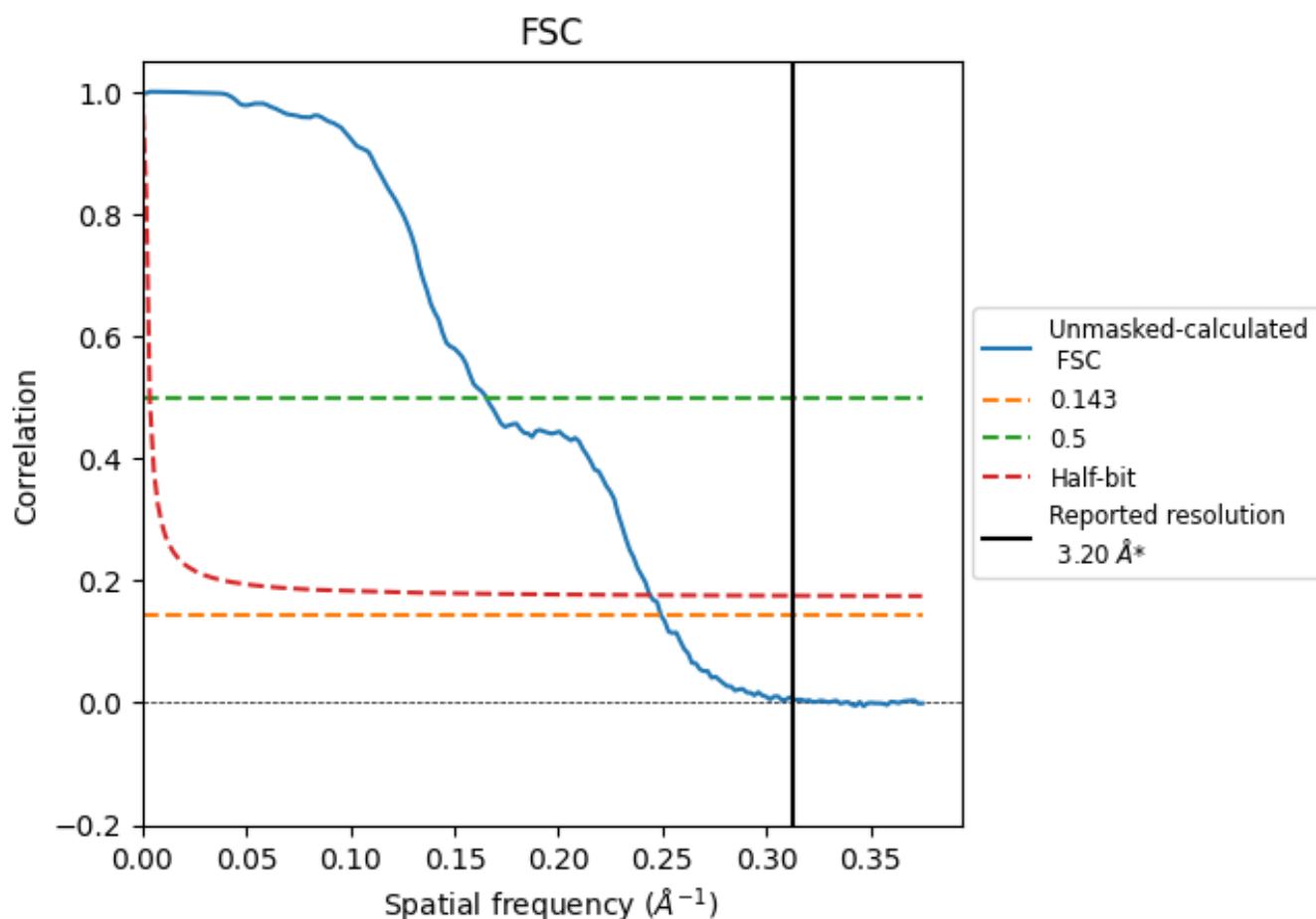


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

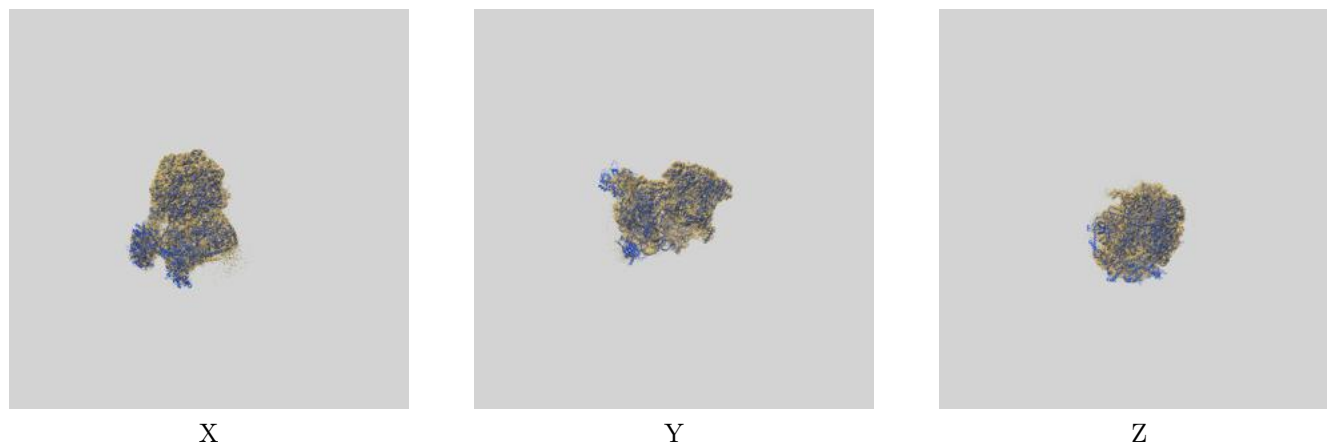
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.20                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 4.01                               | 6.05 | 4.10     |

\*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 4.01 differs from the reported value 3.2 by more than 10 %

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

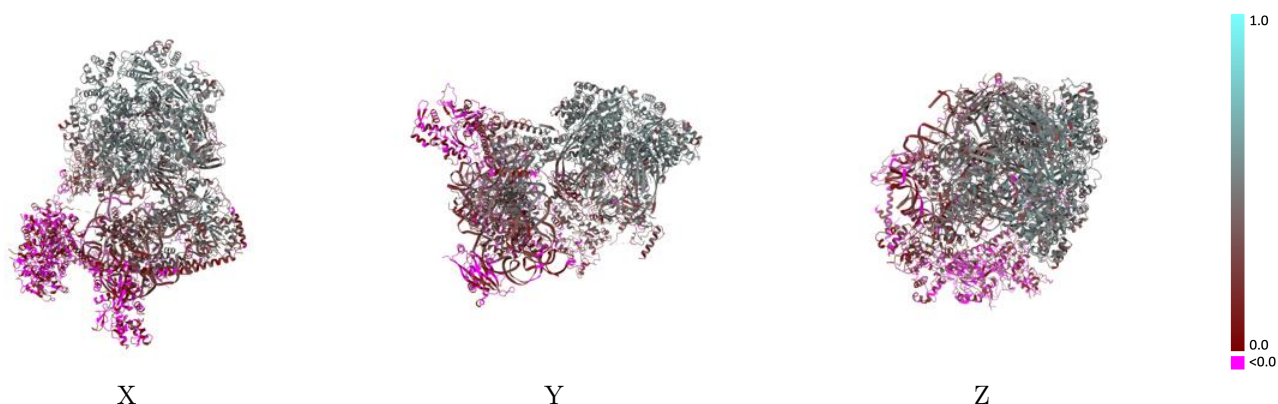
This section contains information regarding the fit between EMDB map EMD-37988 and PDB model 8X19. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

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



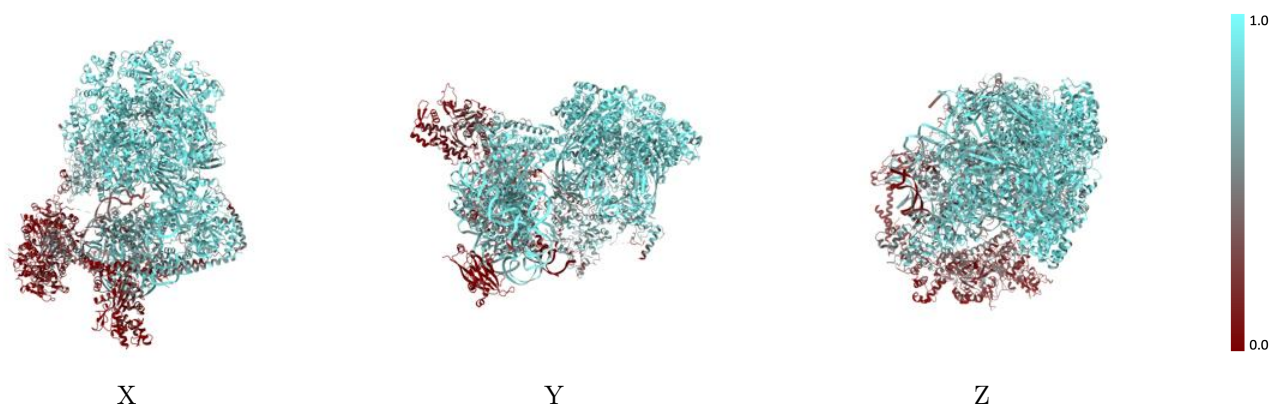
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



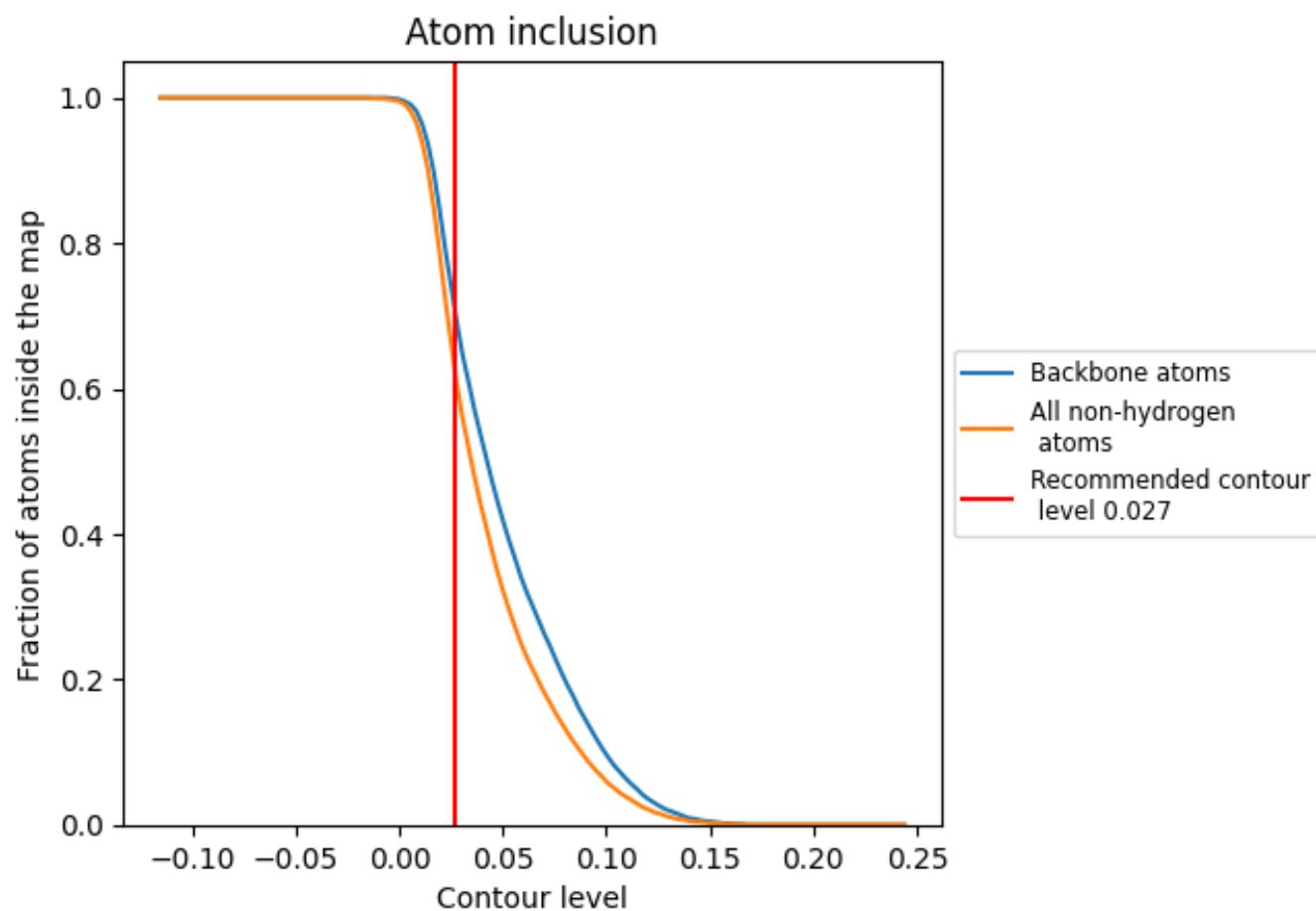
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 62% 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 (0.027) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6220   |  0.2920   |
| A     |  0.6500   |  0.2420   |
| B     |  0.6660   |  0.2500   |
| C     |  0.6640   |  0.2180   |
| D     |  0.7370   |  0.2590   |
| E     |  0.7430   |  0.3420   |
| F     |  0.7460   |  0.3170   |
| G     |  0.8160   |  0.3950   |
| H     |  0.8380   |  0.4060   |
| I     |  0.7210   |  0.3600   |
| J     |  0.4800   |  0.2110   |
| K     |  0.6010   |  0.2190   |
| L     |  0.5320   |  0.1960   |
| M     |  0.8670   |  0.4860   |
| N     |  0.8400  |  0.4560  |
| O     |  0.8280 |  0.4490 |
| P     |  0.8460 |  0.4690 |
| Q     |  0.8370 |  0.4600 |
| R     |  0.8400 |  0.4790 |
| S     |  0.1210 |  0.0340 |
| T     |  0.1710 |  0.0240 |
| U     |  0.1460 |  0.0250 |
| V     |  0.1000 |  0.0420 |
| W     |  0.0160 |  0.0120 |
| X     |  0.7320 |  0.2290 |
| Y     |  0.7400 |  0.2360 |

