



## Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 07:41 AM UTC

PDB ID : 7MKO / pdb\_00007mko  
EMDB ID : EMD-23901  
Title : Escherichia coli RNA polymerase elongation complex  
Authors : Qayyum, M.Z.; Murakami, K.S.  
Deposited on : 2021-04-26  
Resolution : 3.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

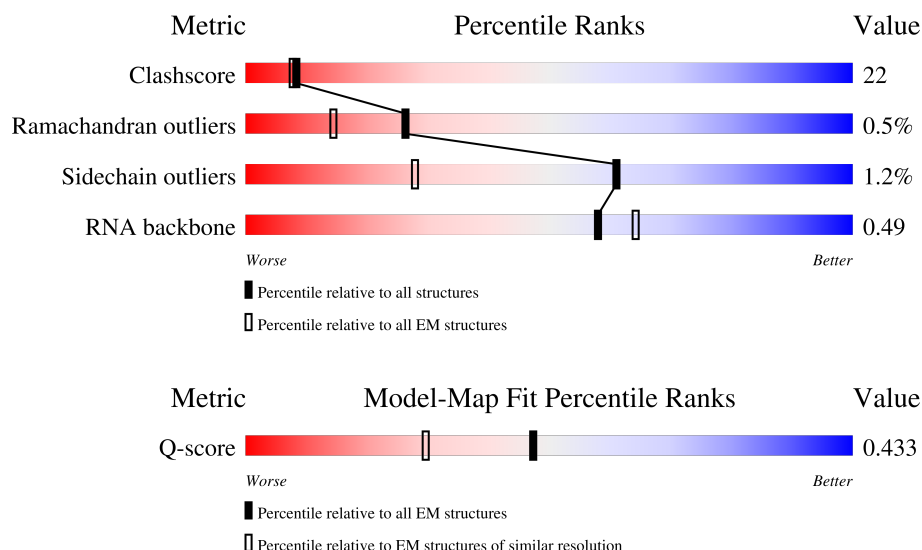
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.15 Å.

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



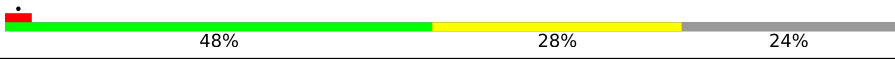
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 14486 ( 2.65 - 3.65 )                                    |

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     | 237    |                  |
| 1   | B     | 237    |                  |
| 2   | C     | 1340   |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 3   | D     | 1363   |  |
| 4   | E     | 91     |  |
| 5   | N     | 29     |  |
| 6   | R     | 11     |  |
| 7   | T     | 29     |  |

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 26269 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 DNA-directed RNA polymerase subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 231      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1794  | 1117 | 318 | 353 | 6 |         |       |
| 1   | B     | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1786  | 1112 | 317 | 351 | 6 |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | C     | 1320     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10414 | 6532 | 1815 | 2024 | 43 |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 3   | D     | 1344     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10419 | 6546 | 1856 | 1967 | 50 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | E     | 69       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 546   | 335 | 105 | 105 | 1 |         |       |

- Molecule 5 is a DNA chain called DNA (29-MER).

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 5   | N     | 22       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 451   | 214 | 89 | 127 | 21 |         |       |

- Molecule 6 is a RNA chain called RNA (20-MER).

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 6   | R     | 11       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 244   | 108 | 50 | 75 | 11 |         |       |

- Molecule 7 is a DNA chain called DNA (29-MER).

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 7   | T     | 29       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 583   | 279 | 99 | 177 | 28 |         |       |

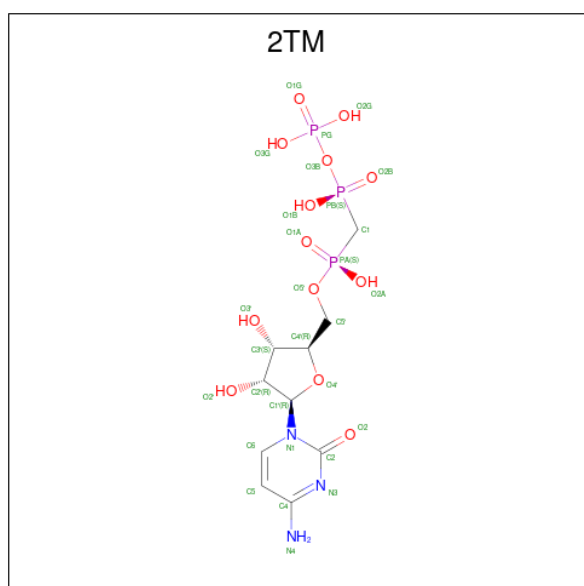
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 8   | D     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 9   | D     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |

- Molecule 10 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (CCD ID: 2TM) (formula: C<sub>10</sub>H<sub>18</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

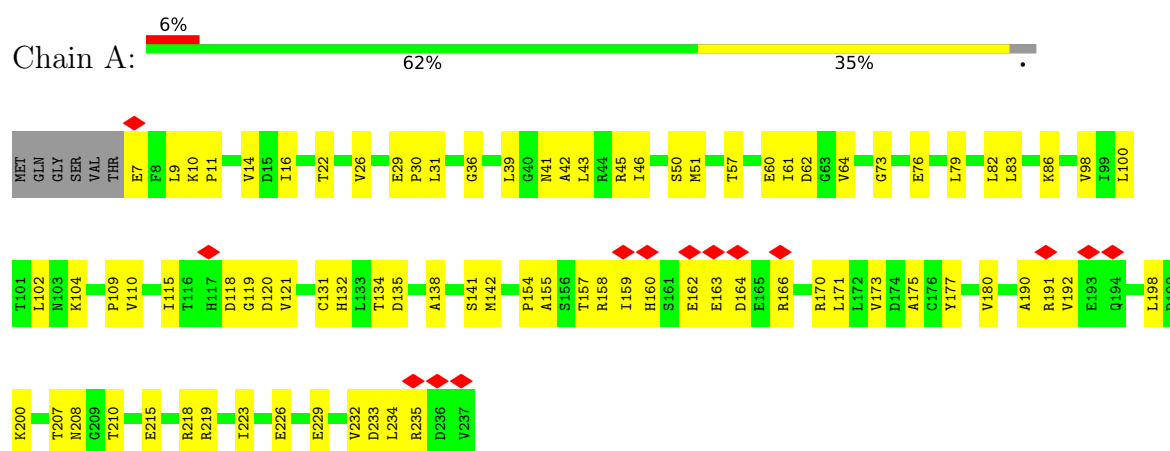


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
|     |       |          | Total | C  | N | O  | P |         |
| 10  | D     | 1        | 29    | 10 | 3 | 13 | 3 | 0       |

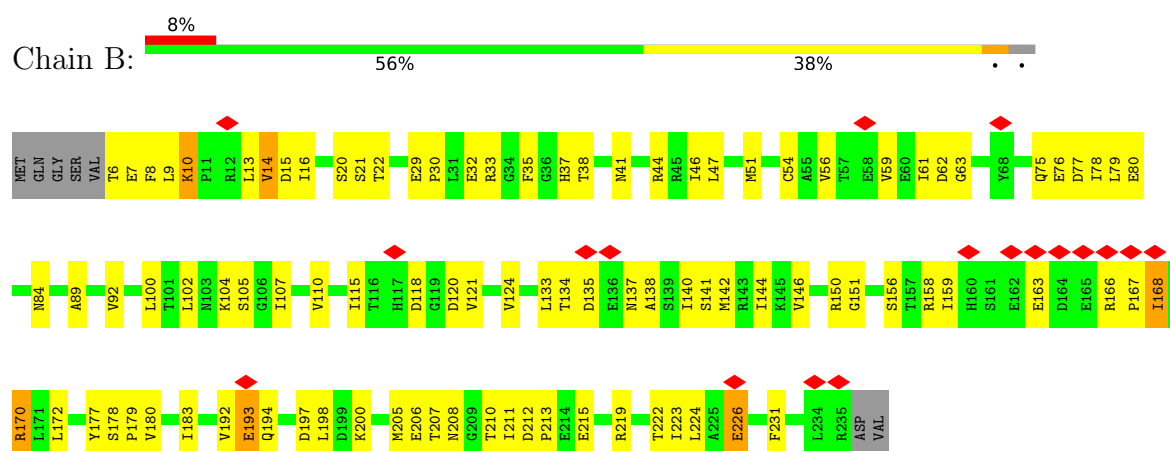
### 3 Residue-property plots [i](#)

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

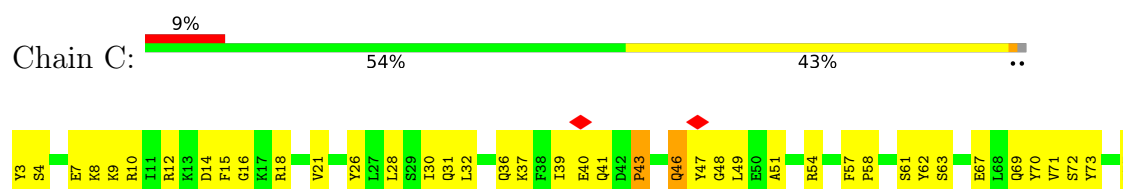
- Molecule 1: DNA-directed RNA polymerase subunit alpha



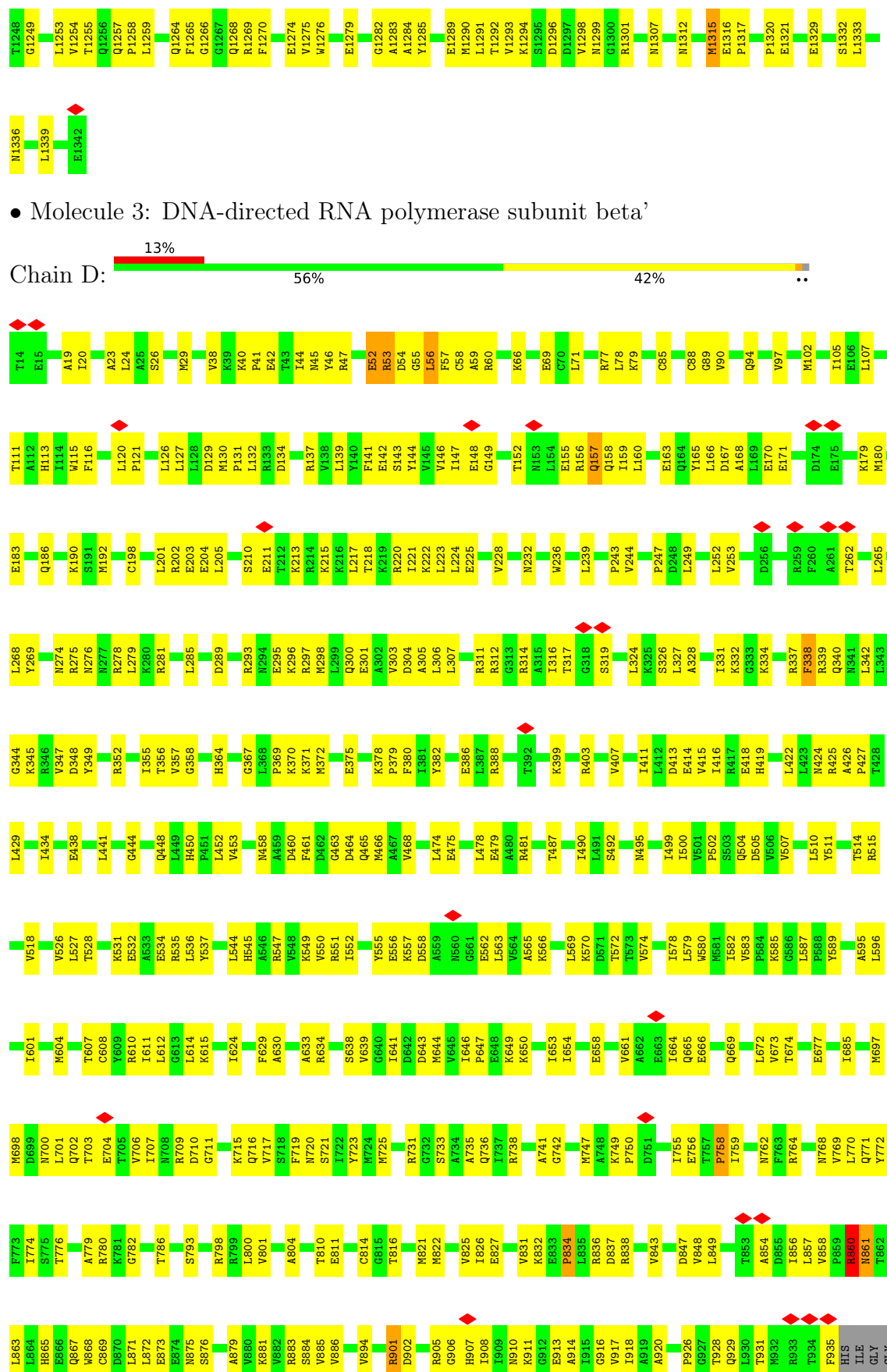
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta







WORLDWIDE  
**PDB**  
PROTEIN DATA BANK



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 256565                                  | 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 ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.204                                   | Depositor |
| Minimum map value                    | -0.111                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.006                                   | Depositor |
| Recommended contour level            | 0.02                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 343.2, 343.2, 343.2                     | wwPDB     |
| Map dimensions                       | 260, 260, 260                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.32, 1.32, 1.32                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 2TM

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     | 0.24         | 0/1816      | 0.51        | 0/2461          |
| 1   | B     | 0.30         | 0/1808      | 0.68        | 4/2450 (0.2%)   |
| 2   | C     | 0.33         | 0/10580     | 0.61        | 4/14274 (0.0%)  |
| 3   | D     | 0.29         | 0/10577     | 0.60        | 4/14284 (0.0%)  |
| 4   | E     | 0.19         | 0/548       | 0.44        | 0/738           |
| 5   | N     | 0.24         | 0/506       | 0.46        | 0/777           |
| 6   | R     | 0.35         | 0/274       | 0.56        | 0/427           |
| 7   | T     | 0.40         | 0/650       | 0.60        | 0/1000          |
| All | All   | 0.30         | 0/26759     | 0.60        | 12/36411 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | C     | 0                   | 2                   |
| 3   | D     | 0                   | 3                   |
| All | All   | 0                   | 5                   |

There are no bond length outliers.

All (12) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3   | D     | 758  | PRO  | CA-N-CD  | -7.91 | 100.93      | 112.00   |
| 1   | B     | 170  | ARG  | CB-CG-CD | 6.70  | 126.72      | 111.30   |
| 1   | B     | 226  | GLU  | N-CA-CB  | 6.50  | 119.67      | 110.12   |
| 2   | C     | 542  | ARG  | CB-CG-CD | -6.33 | 96.75       | 111.30   |
| 2   | C     | 114  | VAL  | N-CA-C   | -6.08 | 104.11      | 113.16   |
| 3   | D     | 1020 | TRP  | CA-CB-CG | 6.08  | 125.14      | 113.60   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | C     | 110 | PRO  | N-CA-C   | -5.76 | 102.16      | 111.14   |
| 2   | C     | 46  | GLN  | CA-CB-CG | 5.51  | 125.12      | 114.10   |
| 1   | B     | 168 | ILE  | CA-C-N   | 5.43  | 130.83      | 122.20   |
| 1   | B     | 168 | ILE  | C-N-CA   | 5.43  | 130.83      | 122.20   |
| 3   | D     | 834 | PRO  | N-CD-CG  | -5.20 | 95.39       | 103.20   |
| 3   | D     | 834 | PRO  | CA-N-CD  | -5.18 | 104.74      | 112.00   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 2   | C     | 236  | LYS  | Peptide |
| 2   | C     | 595  | THR  | Peptide |
| 3   | D     | 1184 | ASP  | Peptide |
| 3   | D     | 860  | ARG  | Peptide |
| 3   | D     | 901  | ARG  | 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     | 1794  | 0        | 1819     | 65      | 0            |
| 1   | B     | 1786  | 0        | 1813     | 84      | 0            |
| 2   | C     | 10414 | 0        | 10420    | 495     | 0            |
| 3   | D     | 10419 | 0        | 10606    | 524     | 0            |
| 4   | E     | 546   | 0        | 565      | 72      | 0            |
| 5   | N     | 451   | 0        | 248      | 9       | 0            |
| 6   | R     | 244   | 0        | 120      | 5       | 0            |
| 7   | T     | 583   | 0        | 329      | 17      | 0            |
| 8   | D     | 1     | 0        | 0        | 0       | 0            |
| 9   | D     | 2     | 0        | 0        | 0       | 0            |
| 10  | D     | 29    | 0        | 14       | 2       | 0            |
| All | All   | 26269 | 0        | 25934    | 1126    | 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 22.

All (1126) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:474:LEU:HD23  | 4:E:28:ARG:CG     | 1.56                     | 1.32              |
| 3:D:910:ASN:ND2   | 4:E:15:ASN:OD1    | 1.74                     | 1.20              |
| 3:D:474:LEU:HD23  | 4:E:28:ARG:HG2    | 1.15                     | 1.08              |
| 3:D:474:LEU:CD2   | 4:E:28:ARG:CG     | 2.35                     | 1.05              |
| 3:D:474:LEU:CD2   | 4:E:28:ARG:HG2    | 1.85                     | 1.04              |
| 3:D:474:LEU:HD23  | 4:E:28:ARG:HG3    | 1.38                     | 1.03              |
| 3:D:905:ARG:HD2   | 4:E:16:ARG:HH11   | 1.24                     | 1.00              |
| 3:D:419:HIS:N     | 4:E:45:LYS:HZ3    | 1.61                     | 0.97              |
| 2:C:560:PRO:HB2   | 3:D:776:THR:HG21  | 1.51                     | 0.93              |
| 2:C:1269:ARG:NH1  | 7:T:16:DA:OP1     | 2.02                     | 0.92              |
| 3:D:1344:LEU:O    | 3:D:1346:GLY:N    | 2.01                     | 0.91              |
| 3:D:419:HIS:N     | 4:E:45:LYS:NZ     | 2.18                     | 0.90              |
| 2:C:1282:GLY:HA3  | 4:E:17:PHE:CE1    | 2.06                     | 0.90              |
| 2:C:525:THR:HG21  | 2:C:687:ARG:HD2   | 1.51                     | 0.89              |
| 3:D:913:GLU:HG2   | 4:E:17:PHE:CE2    | 2.07                     | 0.89              |
| 3:D:111:THR:HG21  | 3:D:303:VAL:HG11  | 1.54                     | 0.89              |
| 2:C:1282:GLY:HA3  | 4:E:17:PHE:HE1    | 1.38                     | 0.89              |
| 2:C:839:VAL:O     | 2:C:886:LYS:NZ    | 2.07                     | 0.88              |
| 2:C:1243:MET:HE1  | 3:D:371:LYS:HD2   | 1.55                     | 0.88              |
| 3:D:1346:GLY:O    | 3:D:1350:ASN:ND2  | 2.06                     | 0.88              |
| 3:D:474:LEU:CD2   | 4:E:28:ARG:HG3    | 2.03                     | 0.87              |
| 3:D:910:ASN:OD1   | 4:E:15:ASN:HA     | 1.59                     | 0.87              |
| 3:D:419:HIS:HB2   | 4:E:45:LYS:NZ     | 1.90                     | 0.87              |
| 3:D:1314:LEU:HB2  | 3:D:1326:GLN:HE22 | 1.38                     | 0.86              |
| 3:D:672:LEU:HD12  | 3:D:673:VAL:HG13  | 1.58                     | 0.85              |
| 1:B:92:VAL:HG12   | 1:B:121:VAL:HG12  | 1.56                     | 0.85              |
| 3:D:120:LEU:HB2   | 3:D:1330:ARG:HH21 | 1.40                     | 0.84              |
| 3:D:615:LYS:NZ    | 4:E:5:THR:HB      | 1.91                     | 0.83              |
| 3:D:419:HIS:H     | 4:E:45:LYS:HZ3    | 1.24                     | 0.83              |
| 2:C:79:VAL:HG13   | 2:C:80:PHE:HD1    | 1.44                     | 0.82              |
| 1:B:168:ILE:O     | 1:B:170:ARG:NH2   | 2.12                     | 0.82              |
| 1:B:167:PRO:HB2   | 1:B:170:ARG:HH21  | 1.45                     | 0.81              |
| 2:C:514:PHE:HZ    | 7:T:21:DT:H5'     | 1.44                     | 0.81              |
| 3:D:438:GLU:OE1   | 4:E:2:ALA:CB      | 2.29                     | 0.81              |
| 2:C:714:VAL:HB    | 2:C:787:PRO:HD2   | 1.62                     | 0.81              |
| 3:D:615:LYS:HZ3   | 4:E:5:THR:HB      | 1.44                     | 0.81              |
| 3:D:438:GLU:OE2   | 4:E:2:ALA:HB1     | 1.82                     | 0.80              |
| 2:C:558:VAL:HG11  | 2:C:573:ASN:HB3   | 1.63                     | 0.80              |
| 3:D:205:LEU:HD21  | 3:D:217:LEU:HB3   | 1.64                     | 0.80              |
| 3:D:418:GLU:O     | 3:D:481:ARG:NH2   | 2.15                     | 0.80              |
| 2:C:1291:LEU:HD11 | 3:D:1351:VAL:HG13 | 1.64                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1330:ARG:NH1  | 7:T:11:DC:OP1     | 2.15                     | 0.79              |
| 3:D:552:ILE:HD11  | 3:D:570:LYS:HG3   | 1.63                     | 0.79              |
| 3:D:1061:VAL:HB   | 3:D:1105:ALA:HB3  | 1.63                     | 0.79              |
| 2:C:533:LEU:HD21  | 2:C:540:ARG:HB3   | 1.66                     | 0.78              |
| 3:D:515:ARG:NH2   | 3:D:717:VAL:O     | 2.17                     | 0.78              |
| 2:C:1058:ARG:NH1  | 2:C:1240:ASP:OD2  | 2.17                     | 0.78              |
| 3:D:1038:THR:HG21 | 3:D:1079:LYS:HD3  | 1.65                     | 0.77              |
| 1:B:134:THR:HG22  | 1:B:135:ASP:H     | 1.50                     | 0.77              |
| 2:C:214:ASN:O     | 2:C:214:ASN:ND2   | 2.17                     | 0.77              |
| 2:C:514:PHE:CZ    | 7:T:21:DT:H5'     | 2.18                     | 0.77              |
| 3:D:337:ARG:O     | 3:D:340:GLN:N     | 2.17                     | 0.76              |
| 3:D:926:PRO:HB3   | 3:D:1246:VAL:HG21 | 1.68                     | 0.76              |
| 2:C:543:ALA:O     | 2:C:548:ARG:NH1   | 2.18                     | 0.76              |
| 2:C:849:GLU:HG3   | 2:C:851:THR:H     | 1.50                     | 0.76              |
| 3:D:910:ASN:CG    | 4:E:15:ASN:OD1    | 2.29                     | 0.75              |
| 3:D:913:GLU:HG2   | 4:E:17:PHE:HE2    | 1.49                     | 0.75              |
| 2:C:542:ARG:HA    | 2:C:542:ARG:NE    | 2.02                     | 0.75              |
| 3:D:419:HIS:HB2   | 4:E:45:LYS:HZ1    | 1.51                     | 0.75              |
| 2:C:692:THR:HG22  | 2:C:693:LEU:H     | 1.51                     | 0.75              |
| 2:C:540:ARG:NH2   | 6:R:17:G:OP2      | 2.20                     | 0.74              |
| 2:C:3:TYR:O       | 2:C:8:LYS:NZ      | 2.21                     | 0.74              |
| 2:C:1101:LEU:HB3  | 3:D:731:ARG:HG3   | 1.69                     | 0.74              |
| 3:D:905:ARG:HD2   | 4:E:16:ARG:NH1    | 2.01                     | 0.74              |
| 3:D:1341:ARG:NH1  | 3:D:1343:GLU:OE2  | 2.20                     | 0.74              |
| 1:A:79:LEU:HD21   | 2:C:693:LEU:HD22  | 1.70                     | 0.74              |
| 2:C:161:LYS:HB3   | 2:C:170:VAL:HG13  | 1.70                     | 0.73              |
| 3:D:826:ILE:HG22  | 3:D:831:VAL:HG12  | 1.70                     | 0.73              |
| 3:D:910:ASN:ND2   | 4:E:15:ASN:CG     | 2.38                     | 0.73              |
| 3:D:334:LYS:HA    | 3:D:339:ARG:HD3   | 1.70                     | 0.73              |
| 1:A:10:LYS:HE3    | 1:B:226:GLU:HB3   | 1.70                     | 0.73              |
| 3:D:438:GLU:CD    | 4:E:2:ALA:HB1     | 2.13                     | 0.73              |
| 1:A:191:ARG:NH1   | 1:A:192:VAL:O     | 2.23                     | 0.72              |
| 2:C:1246:ARG:NH1  | 2:C:1258:PRO:HB2  | 2.03                     | 0.72              |
| 2:C:876:GLU:HG2   | 2:C:927:THR:HG22  | 1.71                     | 0.72              |
| 3:D:388:ARG:HH22  | 3:D:414:GLU:HG2   | 1.55                     | 0.72              |
| 2:C:310:ILE:HG13  | 2:C:311:CYS:H     | 1.54                     | 0.71              |
| 3:D:364:HIS:HB3   | 4:E:4:VAL:HG23    | 1.71                     | 0.71              |
| 1:B:9:LEU:HD21    | 1:B:30:PRO:HG2    | 1.71                     | 0.71              |
| 1:B:215:GLU:OE1   | 1:B:219:ARG:NH1   | 2.22                     | 0.71              |
| 2:C:176:ILE:HD11  | 2:C:428:VAL:HG21  | 1.71                     | 0.71              |
| 2:C:41:GLN:NE2    | 2:C:72:SER:OG     | 2.23                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:542:ARG:HD3   | 5:N:17:DA:C4      | 2.26                     | 0.71              |
| 3:D:418:GLU:HB2   | 4:E:45:LYS:HE2    | 1.73                     | 0.71              |
| 2:C:115:LYS:NZ    | 2:C:485:ASP:OD1   | 2.20                     | 0.71              |
| 2:C:519:ASN:HD21  | 2:C:796:LEU:HD22  | 1.56                     | 0.70              |
| 2:C:1024:GLU:HA   | 2:C:1027:LYS:HE2  | 1.73                     | 0.70              |
| 2:C:1298:VAL:HG12 | 2:C:1301:ARG:HH21 | 1.57                     | 0.70              |
| 3:D:419:HIS:CB    | 4:E:45:LYS:HZ1    | 2.04                     | 0.70              |
| 2:C:434:ASP:OD1   | 2:C:439:LYS:HG3   | 1.91                     | 0.70              |
| 3:D:885:VAL:HG22  | 3:D:1258:ARG:HD2  | 1.74                     | 0.69              |
| 1:B:41:ASN:HD22   | 2:C:1217:THR:HA   | 1.58                     | 0.69              |
| 2:C:1219:GLU:OE1  | 3:D:634:ARG:NH2   | 2.25                     | 0.69              |
| 3:D:1027:VAL:HB   | 3:D:1121:LEU:HB2  | 1.75                     | 0.69              |
| 2:C:821:ARG:HB2   | 2:C:1082:ILE:HD13 | 1.75                     | 0.69              |
| 2:C:1070:HIS:NE2  | 2:C:1114:GLU:OE1  | 2.25                     | 0.69              |
| 3:D:614:LEU:HD23  | 4:E:5:THR:CG2     | 2.23                     | 0.69              |
| 2:C:398:SER:HB2   | 2:C:401:GLY:H     | 1.58                     | 0.69              |
| 1:A:62:ASP:OD2    | 1:A:141:SER:OG    | 2.10                     | 0.68              |
| 2:C:836:LEU:HD21  | 2:C:921:PRO:HD3   | 1.75                     | 0.68              |
| 3:D:426:ALA:HB3   | 3:D:427:PRO:HD3   | 1.75                     | 0.68              |
| 2:C:706:ARG:HG3   | 2:C:793:GLU:HG2   | 1.76                     | 0.68              |
| 3:D:1194:ARG:HD2  | 3:D:1211:SER:HB2  | 1.76                     | 0.68              |
| 10:D:2004:2TM:O2  | 7:T:14:DG:N2      | 2.16                     | 0.68              |
| 1:B:102:LEU:HD13  | 1:B:115:ILE:HD13  | 1.76                     | 0.68              |
| 3:D:1321:SER:OG   | 3:D:1349:GLU:OE1  | 2.11                     | 0.68              |
| 1:A:157:THR:O     | 1:A:160:HIS:ND1   | 2.26                     | 0.68              |
| 2:C:620:ASN:HD21  | 3:D:768:ASN:HB2   | 1.58                     | 0.67              |
| 2:C:808:ASN:H     | 3:D:633:ALA:HB2   | 1.60                     | 0.67              |
| 3:D:218:THR:O     | 3:D:222:LYS:HG2   | 1.93                     | 0.67              |
| 2:C:87:ILE:HG23   | 2:C:932:GLN:HE22  | 1.58                     | 0.67              |
| 1:B:61:ILE:HG22   | 1:B:63:GLY:H      | 1.60                     | 0.67              |
| 3:D:252:LEU:HG    | 3:D:262:THR:HG22  | 1.75                     | 0.67              |
| 3:D:77:ARG:HG3    | 3:D:79:LYS:H      | 1.60                     | 0.67              |
| 2:C:1105:SER:OG   | 3:D:731:ARG:NH2   | 2.28                     | 0.67              |
| 1:B:77:ASP:OD1    | 1:B:78:ILE:N      | 2.29                     | 0.66              |
| 2:C:18:ARG:HE     | 2:C:620:ASN:HA    | 1.59                     | 0.66              |
| 1:B:167:PRO:HG2   | 1:B:170:ARG:HE    | 1.61                     | 0.66              |
| 3:D:137:ARG:HA    | 3:D:142:GLU:OE2   | 1.94                     | 0.66              |
| 3:D:926:PRO:HG3   | 3:D:1248:ILE:HD11 | 1.77                     | 0.66              |
| 3:D:1325:PHE:CZ   | 3:D:1326:GLN:HG3  | 2.30                     | 0.66              |
| 1:A:104:LYS:HD2   | 1:A:110:VAL:HG22  | 1.78                     | 0.66              |
| 1:B:35:PHE:HA     | 1:B:38:THR:HG22   | 1.76                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:647:PRO:HG2   | 3:D:650:LYS:HB2   | 1.78                     | 0.66              |
| 3:D:735:ALA:HA    | 3:D:738:ARG:HD3   | 1.75                     | 0.66              |
| 2:C:689:ALA:HB2   | 2:C:1233:LEU:HD23 | 1.77                     | 0.66              |
| 3:D:364:HIS:CB    | 4:E:4:VAL:HG23    | 2.25                     | 0.66              |
| 3:D:515:ARG:NH2   | 3:D:717:VAL:HG13  | 2.11                     | 0.65              |
| 2:C:15:PHE:HE2    | 2:C:1194:GLU:HB3  | 1.61                     | 0.65              |
| 2:C:772:SER:N     | 2:C:775:GLU:OE1   | 2.26                     | 0.65              |
| 3:D:306:LEU:O     | 3:D:326:SER:OG    | 2.15                     | 0.65              |
| 2:C:32:LEU:HD23   | 2:C:130:MET:HE3   | 1.77                     | 0.65              |
| 2:C:463:GLN:HG2   | 2:C:505:PHE:HB2   | 1.78                     | 0.65              |
| 3:D:357:VAL:HG23  | 3:D:358:GLY:H     | 1.61                     | 0.65              |
| 2:C:841:ARG:HG2   | 2:C:1046:VAL:HG22 | 1.78                     | 0.65              |
| 3:D:141:PHE:HA    | 3:D:180:MET:HE3   | 1.77                     | 0.65              |
| 1:A:180:VAL:HA    | 1:A:207:THR:HG22  | 1.79                     | 0.65              |
| 3:D:905:ARG:CD    | 4:E:16:ARG:HH11   | 2.06                     | 0.65              |
| 2:C:692:THR:HG21  | 2:C:827:ARG:O     | 1.97                     | 0.65              |
| 2:C:841:ARG:N     | 2:C:848:GLU:OE2   | 2.29                     | 0.65              |
| 3:D:700:ASN:O     | 3:D:704:GLU:HB3   | 1.96                     | 0.65              |
| 3:D:798:ARG:NH1   | 3:D:1325:PHE:HB2  | 2.11                     | 0.65              |
| 2:C:839:VAL:HG13  | 2:C:1049:ILE:HG22 | 1.79                     | 0.65              |
| 3:D:281:ARG:HG3   | 3:D:281:ARG:HH11  | 1.61                     | 0.65              |
| 1:B:158:ARG:HB2   | 1:B:172:LEU:HD21  | 1.79                     | 0.64              |
| 2:C:1223:ARG:NH2  | 3:D:719:PHE:O     | 2.25                     | 0.64              |
| 3:D:1031:VAL:HG22 | 3:D:1080:ILE:HD12 | 1.79                     | 0.64              |
| 3:D:217:LEU:O     | 3:D:221:ILE:HD12  | 1.96                     | 0.64              |
| 2:C:912:ASP:O     | 2:C:913:VAL:HG22  | 1.98                     | 0.64              |
| 3:D:134:ASP:HB3   | 3:D:159:ILE:HG13  | 1.79                     | 0.64              |
| 2:C:848:GLU:HG3   | 2:C:886:LYS:HE3   | 1.80                     | 0.64              |
| 2:C:206:ALA:O     | 2:C:209:ILE:HG22  | 1.98                     | 0.64              |
| 3:D:419:HIS:CA    | 4:E:45:LYS:HZ1    | 2.10                     | 0.64              |
| 1:A:100:LEU:HD23  | 1:A:115:ILE:HG21  | 1.79                     | 0.64              |
| 2:C:99:LYS:HD2    | 2:C:118:LYS:HE2   | 1.78                     | 0.64              |
| 2:C:1103:VAL:HG22 | 2:C:1111:GLN:HE21 | 1.63                     | 0.64              |
| 2:C:1329:GLU:OE2  | 3:D:327:LEU:HB3   | 1.98                     | 0.64              |
| 3:D:1061:VAL:HG11 | 3:D:1101:LEU:HB2  | 1.78                     | 0.64              |
| 1:B:84:ASN:OD1    | 3:D:551:ARG:NH2   | 2.31                     | 0.63              |
| 2:C:960:LEU:HB3   | 2:C:1025:PHE:HE1  | 1.62                     | 0.63              |
| 3:D:438:GLU:OE1   | 4:E:2:ALA:HB1     | 1.98                     | 0.63              |
| 3:D:507:VAL:HG23  | 3:D:601:ILE:HD12  | 1.81                     | 0.63              |
| 1:B:124:VAL:HG11  | 1:B:210:THR:HA    | 1.80                     | 0.63              |
| 3:D:1172:LYS:HE3  | 3:D:1189:MET:HB3  | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:105:SER:HA    | 1:B:138:ALA:O     | 1.98                     | 0.63              |
| 2:C:790:ASP:OD1   | 2:C:791:LEU:HD13  | 1.99                     | 0.63              |
| 2:C:1151:LEU:HD22 | 2:C:1198:LEU:HD13 | 1.79                     | 0.63              |
| 1:A:16:ILE:HG23   | 1:A:26:VAL:HG22   | 1.79                     | 0.63              |
| 3:D:1064:SER:OG   | 3:D:1192:LYS:O    | 2.17                     | 0.63              |
| 3:D:337:ARG:O     | 3:D:339:ARG:N     | 2.32                     | 0.63              |
| 1:B:206:GLU:OE2   | 3:D:531:LYS:NZ    | 2.29                     | 0.62              |
| 3:D:364:HIS:CG    | 4:E:4:VAL:HG23    | 2.34                     | 0.62              |
| 3:D:641:ILE:O     | 3:D:764:ARG:NH1   | 2.31                     | 0.62              |
| 2:C:1088:ASP:OD1  | 2:C:1089:GLU:N    | 2.32                     | 0.62              |
| 3:D:1173:ARG:HB2  | 3:D:1192:LYS:HZ3  | 1.64                     | 0.62              |
| 2:C:296:VAL:O     | 2:C:335:THR:OG1   | 2.13                     | 0.62              |
| 2:C:519:ASN:HD21  | 2:C:796:LEU:CD2   | 2.12                     | 0.62              |
| 1:A:11:PRO:HA     | 1:A:30:PRO:HG2    | 1.82                     | 0.62              |
| 3:D:281:ARG:O     | 3:D:285:LEU:HG    | 1.99                     | 0.62              |
| 2:C:185:ASP:OD2   | 2:C:200:ARG:NH2   | 2.26                     | 0.62              |
| 3:D:980:THR:OG1   | 3:D:997:VAL:O     | 2.17                     | 0.62              |
| 3:D:1062:LEU:HB3  | 3:D:1066:GLU:HG3  | 1.82                     | 0.62              |
| 2:C:798:GLN:OE1   | 2:C:827:ARG:HB2   | 2.00                     | 0.61              |
| 2:C:1254:VAL:HG23 | 3:D:249:LEU:HA    | 1.80                     | 0.61              |
| 10:D:2004:2TM:H1  | 10:D:2004:2TM:H10 | 1.81                     | 0.61              |
| 5:N:17:DA:C8      | 5:N:17:DA:H5"     | 2.35                     | 0.61              |
| 3:D:19:ALA:HA     | 3:D:1342:ASP:O    | 1.99                     | 0.61              |
| 3:D:721:SER:O     | 3:D:725:MET:HG3   | 1.99                     | 0.61              |
| 1:B:167:PRO:CB    | 1:B:170:ARG:HH21  | 2.13                     | 0.61              |
| 2:C:202:ARG:HE    | 2:C:204:LEU:HD21  | 1.65                     | 0.61              |
| 3:D:827:GLU:HB2   | 3:D:832:LYS:HD3   | 1.82                     | 0.61              |
| 3:D:978:ARG:HG3   | 3:D:1197:ASN:HB2  | 1.82                     | 0.61              |
| 2:C:1125:GLY:HA3  | 2:C:1179:GLY:HA2  | 1.82                     | 0.61              |
| 1:A:39:LEU:O      | 1:A:43:LEU:HG     | 2.01                     | 0.61              |
| 2:C:43:PRO:O      | 2:C:54:ARG:NH2    | 2.34                     | 0.61              |
| 3:D:1179:PRO:HD2  | 3:D:1184:ASP:HA   | 1.83                     | 0.61              |
| 3:D:45:ASN:C      | 3:D:47:ARG:H      | 2.09                     | 0.61              |
| 3:D:370:LYS:HA    | 3:D:441:LEU:HD12  | 1.82                     | 0.61              |
| 3:D:1056:LEU:HD23 | 3:D:1108:GLN:HE21 | 1.66                     | 0.61              |
| 2:C:557:ARG:NH2   | 2:C:611:GLU:OE1   | 2.34                     | 0.61              |
| 1:B:100:LEU:HD13  | 1:B:115:ILE:HG21  | 1.83                     | 0.60              |
| 2:C:1290:MET:HA   | 2:C:1294:LYS:HG3  | 1.83                     | 0.60              |
| 3:D:399:LYS:HB3   | 3:D:403:ARG:HH22  | 1.66                     | 0.60              |
| 2:C:4:SER:HB3     | 2:C:7:GLU:OE1     | 2.00                     | 0.60              |
| 3:D:556:GLU:OE1   | 3:D:558:ASP:HB2   | 2.01                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:674:THR:HG23  | 3:D:677:GLU:H     | 1.67                     | 0.60              |
| 3:D:1019:ASN:O    | 3:D:1020:TRP:CD1  | 2.54                     | 0.60              |
| 3:D:555:TYR:CE1   | 3:D:565:ALA:HB2   | 2.37                     | 0.60              |
| 3:D:1238:GLN:NE2  | 3:D:1248:ILE:O    | 2.31                     | 0.60              |
| 3:D:26:SER:HB3    | 3:D:29:MET:HG3    | 1.81                     | 0.60              |
| 2:C:243:PRO:HB3   | 2:C:277:LEU:HD13  | 1.84                     | 0.60              |
| 3:D:382:TYR:O     | 3:D:386:GLU:HG2   | 2.02                     | 0.60              |
| 2:C:304:GLU:OE1   | 2:C:330:HIS:NE2   | 2.25                     | 0.60              |
| 2:C:411:ARG:NH2   | 2:C:427:ASP:OD2   | 2.35                     | 0.60              |
| 2:C:836:LEU:HB3   | 2:C:918:LEU:HD21  | 1.83                     | 0.60              |
| 1:A:42:ALA:O      | 1:A:46:ILE:HG12   | 2.02                     | 0.59              |
| 1:B:33:ARG:NH1    | 2:C:1081:PRO:HG3  | 2.17                     | 0.59              |
| 1:B:41:ASN:ND2    | 2:C:1217:THR:HA   | 2.18                     | 0.59              |
| 2:C:14:ASP:HA     | 2:C:1183:ALA:HB3  | 1.84                     | 0.59              |
| 3:D:526:VAL:HG12  | 3:D:549:LYS:HB2   | 1.85                     | 0.59              |
| 2:C:80:PHE:HE2    | 2:C:88:ARG:CZ     | 2.16                     | 0.59              |
| 2:C:688:GLN:HB2   | 2:C:1235:LEU:HD22 | 1.83                     | 0.59              |
| 3:D:804:ALA:O     | 3:D:916:GLY:HA3   | 2.02                     | 0.59              |
| 3:D:978:ARG:HD3   | 3:D:999:TYR:HB2   | 1.83                     | 0.59              |
| 2:C:36:GLN:O      | 2:C:40:GLU:HG3    | 2.03                     | 0.59              |
| 3:D:514:THR:OG1   | 3:D:595:ALA:O     | 2.20                     | 0.59              |
| 2:C:338:THR:HB    | 2:C:345:PRO:HG3   | 1.84                     | 0.59              |
| 2:C:890:LYS:HZ3   | 2:C:911:SER:N     | 2.00                     | 0.59              |
| 2:C:1023:HIS:O    | 2:C:1026:GLU:HG3  | 2.03                     | 0.59              |
| 2:C:221:LEU:HD11  | 2:C:314:ASN:HB2   | 1.85                     | 0.59              |
| 1:B:167:PRO:HG2   | 1:B:170:ARG:NE    | 2.18                     | 0.59              |
| 2:C:590:PRO:HB2   | 2:C:655:VAL:HG21  | 1.83                     | 0.59              |
| 3:D:120:LEU:HB3   | 3:D:121:PRO:HD3   | 1.83                     | 0.59              |
| 3:D:380:PHE:HB3   | 3:D:415:VAL:HG21  | 1.84                     | 0.59              |
| 2:C:88:ARG:HB2    | 2:C:88:ARG:NH1    | 2.18                     | 0.59              |
| 2:C:98:VAL:HG11   | 2:C:124:MET:SD    | 2.43                     | 0.59              |
| 3:D:1110:GLU:HG2  | 3:D:1111:ASP:H    | 1.67                     | 0.59              |
| 3:D:742:GLY:O     | 3:D:762:ASN:HB3   | 2.03                     | 0.58              |
| 3:D:827:GLU:O     | 3:D:832:LYS:NZ    | 2.22                     | 0.58              |
| 2:C:1246:ARG:HH12 | 2:C:1258:PRO:HB2  | 1.65                     | 0.58              |
| 3:D:755:ILE:HD12  | 3:D:755:ILE:H     | 1.68                     | 0.58              |
| 3:D:1001:ALA:HB1  | 3:D:1020:TRP:NE1  | 2.19                     | 0.58              |
| 1:B:44:ARG:HA     | 1:B:183:ILE:HD13  | 1.85                     | 0.58              |
| 3:D:913:GLU:CD    | 4:E:17:PHE:HZ     | 2.11                     | 0.58              |
| 1:A:82:LEU:HD11   | 1:A:171:LEU:HD13  | 1.86                     | 0.58              |
| 2:C:229:ILE:HD13  | 2:C:334:GLU:OE1   | 2.02                     | 0.58              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:399:LYS:HB3   | 3:D:403:ARG:NH2  | 2.18                     | 0.58              |
| 3:D:532:GLU:HA    | 3:D:535:ARG:HD3  | 1.85                     | 0.58              |
| 2:C:211:ARG:NH1   | 2:C:217:THR:OG1  | 2.36                     | 0.58              |
| 2:C:1298:VAL:HG12 | 2:C:1301:ARG:NH2 | 2.19                     | 0.58              |
| 3:D:111:THR:O     | 3:D:239:LEU:N    | 2.32                     | 0.58              |
| 3:D:107:LEU:HA    | 3:D:276:ASN:HD21 | 1.69                     | 0.58              |
| 3:D:884:SER:OG    | 3:D:1254:GLU:OE1 | 2.21                     | 0.58              |
| 1:A:109:PRO:HB3   | 1:A:132:HIS:CE1  | 2.39                     | 0.58              |
| 3:D:275:ARG:HH11  | 3:D:298:MET:HB3  | 1.68                     | 0.58              |
| 3:D:913:GLU:HG2   | 4:E:17:PHE:CZ    | 2.37                     | 0.58              |
| 2:C:218:GLU:HG3   | 2:C:299:LYS:HA   | 1.86                     | 0.58              |
| 2:C:799:ASN:HB3   | 2:C:1231:TYR:HD1 | 1.68                     | 0.58              |
| 1:B:219:ARG:O     | 1:B:223:ILE:HG13 | 2.04                     | 0.57              |
| 2:C:189:ASP:OD1   | 2:C:193:ASN:N    | 2.32                     | 0.57              |
| 2:C:550:VAL:H     | 3:D:780:ARG:HD2  | 1.68                     | 0.57              |
| 1:B:205:MET:HG2   | 1:B:213:PRO:HB3  | 1.84                     | 0.57              |
| 2:C:85:CYS:SG     | 2:C:90:VAL:HG23  | 2.44                     | 0.57              |
| 2:C:812:PHE:HA    | 3:D:505:ASP:OD2  | 2.05                     | 0.57              |
| 3:D:961:SER:OG    | 3:D:981:GLU:HB3  | 2.03                     | 0.57              |
| 2:C:558:VAL:CG1   | 2:C:573:ASN:HB3  | 2.34                     | 0.57              |
| 3:D:928:THR:O     | 3:D:931:THR:HG22 | 2.04                     | 0.57              |
| 1:B:20:SER:O      | 1:B:22:THR:N     | 2.37                     | 0.57              |
| 3:D:289:ASP:OD2   | 3:D:293:ARG:HD2  | 2.04                     | 0.57              |
| 2:C:705:GLU:HB3   | 2:C:794:LEU:H    | 1.69                     | 0.57              |
| 3:D:314:ARG:HH21  | 3:D:316:ILE:HD11 | 1.69                     | 0.57              |
| 3:D:514:THR:HG21  | 3:D:596:LEU:HD12 | 1.87                     | 0.57              |
| 3:D:528:THR:N     | 3:D:532:GLU:OE2  | 2.23                     | 0.57              |
| 3:D:1067:ARG:HH21 | 3:D:1076:PRO:HD2 | 1.70                     | 0.57              |
| 3:D:1162:ILE:HD11 | 3:D:1201:GLY:HA2 | 1.87                     | 0.57              |
| 3:D:1327:GLU:HG3  | 3:D:1330:ARG:HD2 | 1.87                     | 0.57              |
| 3:D:419:HIS:CB    | 4:E:45:LYS:NZ    | 2.63                     | 0.57              |
| 2:C:67:GLU:OE1    | 2:C:69:GLN:HG3   | 2.05                     | 0.57              |
| 2:C:755:LYS:O     | 2:C:757:THR:HG23 | 2.05                     | 0.57              |
| 2:C:870:ILE:HG23  | 2:C:884:VAL:HG22 | 1.87                     | 0.57              |
| 2:C:12:ARG:NH1    | 2:C:1182:ILE:O   | 2.36                     | 0.57              |
| 2:C:657:THR:HG21  | 2:C:1188:ASP:HB2 | 1.87                     | 0.57              |
| 3:D:1019:ASN:O    | 3:D:1020:TRP:HD1 | 1.88                     | 0.57              |
| 2:C:542:ARG:NH1   | 5:N:17:DA:C2     | 2.72                     | 0.56              |
| 2:C:1333:LEU:HD22 | 3:D:307:LEU:HD22 | 1.85                     | 0.56              |
| 3:D:1263:LYS:NZ   | 3:D:1315:ALA:HB1 | 2.19                     | 0.56              |
| 2:C:143:ARG:HH21  | 7:T:21:DT:H4'    | 1.70                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:678:ARG:NH2   | 2:C:1071:GLY:O    | 2.38                     | 0.56              |
| 2:C:930:ASP:OD1   | 2:C:931:VAL:N     | 2.38                     | 0.56              |
| 3:D:487:THR:HG21  | 4:E:4:VAL:HG22    | 1.87                     | 0.56              |
| 3:D:831:VAL:HG13  | 3:D:992:LYS:HE3   | 1.87                     | 0.56              |
| 3:D:487:THR:HG21  | 4:E:4:VAL:CG2     | 2.35                     | 0.56              |
| 3:D:458:ASN:HD22  | 3:D:929:GLN:HE22  | 1.53                     | 0.56              |
| 3:D:1179:PRO:HG2  | 3:D:1182:GLY:O    | 2.05                     | 0.56              |
| 3:D:1325:PHE:CE1  | 3:D:1326:GLN:HG3  | 2.39                     | 0.56              |
| 1:A:135:ASP:HB3   | 1:A:138:ALA:HB2   | 1.88                     | 0.56              |
| 2:C:478:ARG:NH2   | 2:C:479:LEU:HA    | 2.20                     | 0.56              |
| 2:C:589:THR:HG23  | 2:C:591:TYR:CE2   | 2.40                     | 0.56              |
| 3:D:782:GLY:O     | 3:D:786:THR:HG23  | 2.06                     | 0.56              |
| 3:D:798:ARG:HH12  | 3:D:1325:PHE:HB2  | 1.69                     | 0.56              |
| 3:D:349:TYR:HE2   | 3:D:379:PRO:HG3   | 1.69                     | 0.56              |
| 1:A:82:LEU:HD23   | 1:A:173:VAL:HG22  | 1.87                     | 0.56              |
| 2:C:83:GLN:O      | 2:C:87:ILE:HG13   | 2.05                     | 0.56              |
| 2:C:1109:ILE:HD12 | 3:D:644:MET:HE1   | 1.88                     | 0.56              |
| 2:C:802:VAL:HG12  | 2:C:1096:ILE:HB   | 1.87                     | 0.56              |
| 2:C:199:ASP:O     | 2:C:200:ARG:NE    | 2.31                     | 0.56              |
| 2:C:1085:MET:HE1  | 2:C:1097:VAL:HG23 | 1.88                     | 0.56              |
| 3:D:478:LEU:HB3   | 4:E:20:VAL:HG13   | 1.87                     | 0.56              |
| 3:D:1327:GLU:HG3  | 3:D:1330:ARG:CD   | 2.36                     | 0.56              |
| 1:B:104:LYS:HG2   | 1:B:110:VAL:HG22  | 1.87                     | 0.55              |
| 2:C:1259:LEU:O    | 2:C:1266:GLY:HA2  | 2.06                     | 0.55              |
| 3:D:141:PHE:CD1   | 3:D:297:ARG:HG3   | 2.41                     | 0.55              |
| 1:A:131:CYS:SG    | 1:A:132:HIS:N     | 2.79                     | 0.55              |
| 2:C:660:VAL:HG21  | 3:D:769:VAL:CG1   | 2.36                     | 0.55              |
| 2:C:987:GLU:HG3   | 2:C:988:LYS:H     | 1.71                     | 0.55              |
| 3:D:528:THR:HG22  | 3:D:532:GLU:CD    | 2.32                     | 0.55              |
| 1:A:14:VAL:HG21   | 1:A:29:GLU:HG2    | 1.87                     | 0.55              |
| 2:C:80:PHE:HD2    | 2:C:84:GLU:HG3    | 1.71                     | 0.55              |
| 3:D:213:LYS:O     | 3:D:217:LEU:HD23  | 2.07                     | 0.55              |
| 3:D:902:ASP:H     | 3:D:1251:LYS:HZ3  | 1.54                     | 0.55              |
| 1:A:60:GLU:OE2    | 1:A:170:ARG:NE    | 2.33                     | 0.55              |
| 2:C:237:LEU:HD11  | 2:C:322:LEU:HD21  | 1.87                     | 0.55              |
| 2:C:842:ASP:HB2   | 2:C:1047:LEU:HD21 | 1.87                     | 0.55              |
| 2:C:62:TYR:HD2    | 2:C:480:SER:HG    | 1.53                     | 0.55              |
| 2:C:221:LEU:HD22  | 2:C:336:LEU:HD11  | 1.89                     | 0.55              |
| 3:D:407:VAL:O     | 3:D:411:ILE:HG12  | 2.06                     | 0.55              |
| 3:D:1078:LEU:HD13 | 3:D:1101:LEU:HD21 | 1.89                     | 0.55              |
| 3:D:1158:GLU:HG3  | 3:D:1186:TYR:CZ   | 2.42                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:180:MET:HE2   | 3:D:293:ARG:NH2   | 2.22                     | 0.55              |
| 3:D:556:GLU:HG2   | 3:D:566:LYS:NZ    | 2.21                     | 0.55              |
| 3:D:885:VAL:HG23  | 3:D:894:VAL:HG11  | 1.87                     | 0.55              |
| 1:A:162:GLU:OE1   | 1:A:162:GLU:N     | 2.40                     | 0.55              |
| 2:C:696:ASP:OD1   | 2:C:697:LYS:N     | 2.36                     | 0.55              |
| 3:D:857:LEU:HD11  | 3:D:871:LEU:HD21  | 1.88                     | 0.55              |
| 3:D:848:VAL:HG22  | 3:D:858:VAL:HG22  | 1.88                     | 0.55              |
| 2:C:30:ILE:HD11   | 2:C:575:LEU:HD13  | 1.88                     | 0.54              |
| 2:C:685:MET:SD    | 2:C:1073:LYS:HG2  | 2.47                     | 0.54              |
| 2:C:960:LEU:O     | 2:C:963:GLU:HG3   | 2.08                     | 0.54              |
| 2:C:1223:ARG:HH12 | 3:D:719:PHE:HB3   | 1.71                     | 0.54              |
| 3:D:654:ILE:O     | 3:D:658:GLU:HG3   | 2.07                     | 0.54              |
| 2:C:629:PHE:HB2   | 2:C:647:ARG:HD2   | 1.87                     | 0.54              |
| 2:C:870:ILE:HG21  | 2:C:931:VAL:HG11  | 1.87                     | 0.54              |
| 3:D:1072:LYS:O    | 3:D:1075:ARG:NH1  | 2.40                     | 0.54              |
| 1:A:155:ALA:O     | 1:A:158:ARG:HG2   | 2.07                     | 0.54              |
| 2:C:575:LEU:HD21  | 2:C:579:ALA:HB3   | 1.89                     | 0.54              |
| 2:C:716:ALA:HB3   | 2:C:784:ALA:HB3   | 1.90                     | 0.54              |
| 2:C:1033:ARG:HH12 | 2:C:1037:THR:HG21 | 1.72                     | 0.54              |
| 3:D:527:LEU:HD21  | 3:D:536:LEU:HD12  | 1.89                     | 0.54              |
| 3:D:1005:LYS:HD2  | 3:D:1017:VAL:HG23 | 1.88                     | 0.54              |
| 1:B:118:ASP:HB2   | 1:B:121:VAL:HG22  | 1.89                     | 0.54              |
| 3:D:418:GLU:CB    | 4:E:45:LYS:HE2    | 2.38                     | 0.54              |
| 3:D:972:LYS:HE2   | 3:D:1003:LEU:HB3  | 1.88                     | 0.54              |
| 3:D:1279:GLN:NE2  | 3:D:1317:GLU:HG2  | 2.22                     | 0.54              |
| 2:C:515:MET:HE3   | 2:C:523:GLU:HG2   | 1.88                     | 0.54              |
| 2:C:964:LEU:HD11  | 2:C:1025:PHE:CE1  | 2.42                     | 0.54              |
| 3:D:129:ASP:HB2   | 3:D:220:ARG:CZ    | 2.38                     | 0.54              |
| 2:C:423:ASP:HA    | 2:C:426:ILE:HG12  | 1.89                     | 0.54              |
| 2:C:144:VAL:HG21  | 2:C:515:MET:HG3   | 1.90                     | 0.54              |
| 1:B:192:VAL:O     | 1:B:194:GLN:N     | 2.37                     | 0.54              |
| 2:C:393:ASP:OD1   | 2:C:394:ARG:N     | 2.40                     | 0.54              |
| 2:C:624:ASP:O     | 2:C:626:GLU:N     | 2.40                     | 0.54              |
| 1:A:164:ASP:CG    | 1:A:166:ARG:HG2   | 2.33                     | 0.53              |
| 2:C:310:ILE:HG13  | 2:C:311:CYS:N     | 2.23                     | 0.53              |
| 3:D:518:VAL:O     | 3:D:547:ARG:NH2   | 2.36                     | 0.53              |
| 2:C:692:THR:HG22  | 2:C:693:LEU:N     | 2.20                     | 0.53              |
| 2:C:947:GLU:O     | 2:C:950:GLU:HG3   | 2.07                     | 0.53              |
| 2:C:1257:GLN:NE2  | 3:D:345:LYS:HG2   | 2.24                     | 0.53              |
| 3:D:269:TYR:CE1   | 3:D:306:LEU:HD21  | 2.43                     | 0.53              |
| 3:D:527:LEU:HD22  | 3:D:532:GLU:HG3   | 1.89                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:886:VAL:HA    | 3:D:1258:ARG:HG3  | 1.90                     | 0.53              |
| 3:D:1322:ALA:HB3  | 3:D:1331:VAL:HG21 | 1.90                     | 0.53              |
| 2:C:348:SER:O     | 2:C:352:ARG:HG2   | 2.08                     | 0.53              |
| 2:C:1269:ARG:NH2  | 3:D:344:GLY:HA3   | 2.23                     | 0.53              |
| 3:D:367:GLY:HA3   | 3:D:448:GLN:HB2   | 1.91                     | 0.53              |
| 3:D:860:ARG:HG3   | 3:D:861:ASN:H     | 1.72                     | 0.53              |
| 2:C:229:ILE:HB    | 2:C:240:GLU:HB3   | 1.89                     | 0.53              |
| 2:C:666:SER:HA    | 2:C:1186:VAL:HG11 | 1.88                     | 0.53              |
| 3:D:41:PRO:HG3    | 3:D:274:ASN:OD1   | 2.09                     | 0.53              |
| 3:D:863:LEU:HD11  | 3:D:901:ARG:HB3   | 1.89                     | 0.53              |
| 2:C:521:LEU:HD21  | 2:C:664:GLY:HA2   | 1.91                     | 0.53              |
| 2:C:524:ILE:HG21  | 2:C:708:VAL:HG13  | 1.91                     | 0.53              |
| 2:C:1013:GLN:O    | 2:C:1016:GLU:HG2  | 2.09                     | 0.53              |
| 3:D:59:ALA:HB3    | 3:D:71:LEU:HD11   | 1.90                     | 0.53              |
| 3:D:211:GLU:HG3   | 3:D:215:LYS:NZ    | 2.23                     | 0.53              |
| 3:D:268:LEU:HD21  | 3:D:324:LEU:HD11  | 1.89                     | 0.53              |
| 3:D:311:ARG:O     | 3:D:312:ARG:HD3   | 2.09                     | 0.53              |
| 3:D:1063:ASP:HB2  | 3:D:1103:GLY:HA2  | 1.90                     | 0.53              |
| 4:E:42:GLU:OE1    | 4:E:42:GLU:N      | 2.42                     | 0.53              |
| 1:A:22:THR:HB     | 1:A:207:THR:O     | 2.08                     | 0.53              |
| 2:C:149:LEU:HB2   | 2:C:530:ILE:HG22  | 1.90                     | 0.53              |
| 1:A:229:GLU:O     | 1:A:232:VAL:HG22  | 2.09                     | 0.53              |
| 3:D:419:HIS:N     | 4:E:45:LYS:HZ1    | 2.07                     | 0.53              |
| 3:D:749:LYS:HB3   | 3:D:750:PRO:HD2   | 1.90                     | 0.53              |
| 3:D:1264:ALA:HB2  | 3:D:1280:VAL:HG22 | 1.91                     | 0.53              |
| 3:D:1280:VAL:O    | 3:D:1284:ARG:HG2  | 2.09                     | 0.53              |
| 1:B:163:GLU:N     | 1:B:163:GLU:OE1   | 2.42                     | 0.53              |
| 2:C:230:PHE:HE2   | 2:C:335:THR:HG21  | 1.74                     | 0.53              |
| 2:C:256:GLU:HA    | 2:C:261:VAL:HA    | 1.90                     | 0.53              |
| 3:D:902:ASP:H     | 3:D:1251:LYS:NZ   | 2.07                     | 0.53              |
| 2:C:890:LYS:HD3   | 2:C:913:VAL:HG22  | 1.90                     | 0.53              |
| 2:C:813:GLU:HB2   | 3:D:461:PHE:CD2   | 2.45                     | 0.52              |
| 2:C:1077:SER:HB2  | 3:D:357:VAL:HG22  | 1.90                     | 0.52              |
| 3:D:24:LEU:HD12   | 3:D:232:ASN:HB3   | 1.91                     | 0.52              |
| 3:D:55:GLY:H      | 3:D:58:CYS:HB2    | 1.73                     | 0.52              |
| 3:D:220:ARG:O     | 3:D:224:LEU:HD23  | 2.09                     | 0.52              |
| 1:A:234:LEU:HD23  | 1:B:16:ILE:HD11   | 1.91                     | 0.52              |
| 2:C:1298:VAL:HG23 | 2:C:1299:ASN:H    | 1.74                     | 0.52              |
| 3:D:265:LEU:HD21  | 3:D:327:LEU:HG    | 1.90                     | 0.52              |
| 3:D:972:LYS:NZ    | 3:D:974:VAL:HA    | 2.24                     | 0.52              |
| 2:C:934:PHE:HD2   | 2:C:1049:ILE:HD11 | 1.74                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1296:ASP:OD2  | 2:C:1321:GLU:N    | 2.43                     | 0.52              |
| 3:D:1045:THR:O    | 3:D:1046:ILE:HD13 | 2.10                     | 0.52              |
| 2:C:521:LEU:HD22  | 2:C:667:LEU:HD12  | 1.92                     | 0.52              |
| 3:D:572:THR:HG21  | 3:D:589:TYR:CE2   | 2.45                     | 0.52              |
| 3:D:1170:LYS:HD2  | 3:D:1174:ARG:HH12 | 1.75                     | 0.52              |
| 3:D:1205:GLU:OE2  | 3:D:1206:ARG:HG2  | 2.09                     | 0.52              |
| 2:C:660:VAL:HG21  | 3:D:769:VAL:HG13  | 1.91                     | 0.52              |
| 2:C:677:ASN:ND2   | 3:D:779:ALA:HB1   | 2.25                     | 0.52              |
| 3:D:982:LEU:HD23  | 3:D:997:VAL:HB    | 1.91                     | 0.52              |
| 3:D:1279:GLN:HE22 | 3:D:1317:GLU:HG2  | 1.75                     | 0.52              |
| 2:C:540:ARG:O     | 2:C:548:ARG:NH2   | 2.43                     | 0.52              |
| 3:D:450:HIS:CE1   | 3:D:452:LEU:HB2   | 2.45                     | 0.52              |
| 2:C:542:ARG:NE    | 2:C:542:ARG:CA    | 2.70                     | 0.52              |
| 2:C:845:LEU:HD21  | 2:C:890:LYS:C     | 2.34                     | 0.52              |
| 3:D:424:ASN:OD1   | 3:D:425:ARG:N     | 2.42                     | 0.52              |
| 3:D:875:ASN:CG    | 3:D:876:SER:H     | 2.18                     | 0.52              |
| 2:C:46:GLN:O      | 2:C:51:ALA:HB2    | 2.10                     | 0.52              |
| 3:D:703:THR:HG22  | 3:D:703:THR:O     | 2.09                     | 0.52              |
| 2:C:570:GLY:O     | 2:C:573:ASN:ND2   | 2.43                     | 0.52              |
| 3:D:419:HIS:CA    | 4:E:45:LYS:NZ     | 2.69                     | 0.52              |
| 1:B:89:ALA:O      | 1:B:124:VAL:HG22  | 2.09                     | 0.52              |
| 1:B:170:ARG:HG3   | 1:B:170:ARG:HH11  | 1.74                     | 0.52              |
| 3:D:198:CYS:SG    | 3:D:202:ARG:NH1   | 2.83                     | 0.52              |
| 3:D:275:ARG:NH1   | 3:D:298:MET:HB3   | 2.25                     | 0.52              |
| 3:D:355:ILE:HG21  | 3:D:466:MET:SD    | 2.50                     | 0.52              |
| 1:B:180:VAL:HG12  | 1:B:205:MET:HE3   | 1.90                     | 0.51              |
| 2:C:257:ALA:HB3   | 2:C:262:TYR:CE2   | 2.45                     | 0.51              |
| 2:C:954:LYS:NZ    | 2:C:958:LYS:HD2   | 2.25                     | 0.51              |
| 2:C:1246:ARG:HH21 | 2:C:1249:GLY:N    | 2.08                     | 0.51              |
| 4:E:24:ALA:O      | 4:E:28:ARG:HG3    | 2.10                     | 0.51              |
| 1:B:170:ARG:HG3   | 1:B:170:ARG:NH1   | 2.24                     | 0.51              |
| 2:C:833:ILE:HA    | 2:C:1054:LEU:O    | 2.10                     | 0.51              |
| 2:C:1123:GLY:HA3  | 2:C:1204:LEU:HD11 | 1.92                     | 0.51              |
| 3:D:147:ILE:HG13  | 3:D:147:ILE:O     | 2.10                     | 0.51              |
| 3:D:179:LYS:NZ    | 3:D:183:GLU:HG2   | 2.25                     | 0.51              |
| 3:D:810:THR:O     | 3:D:911:LYS:HE3   | 2.10                     | 0.51              |
| 3:D:955:LYS:HE2   | 3:D:1012:ALA:HA   | 1.91                     | 0.51              |
| 3:D:1314:LEU:HB2  | 3:D:1326:GLN:NE2  | 2.18                     | 0.51              |
| 2:C:297:VAL:HB    | 2:C:317:LEU:HD11  | 1.92                     | 0.51              |
| 3:D:202:ARG:HH22  | 3:D:225:GLU:CD    | 2.19                     | 0.51              |
| 1:B:6:THR:OG1     | 1:B:7:GLU:N       | 2.40                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:579:LEU:O     | 3:D:582:ILE:HG12  | 2.10                     | 0.51              |
| 1:B:59:VAL:HG23   | 1:B:144:ILE:HG13  | 1.91                     | 0.51              |
| 2:C:1017:GLN:O    | 2:C:1021:LEU:HD23 | 2.10                     | 0.51              |
| 3:D:913:GLU:OE2   | 4:E:17:PHE:HZ     | 1.93                     | 0.51              |
| 3:D:1239:ASP:OD1  | 3:D:1242:ARG:NH1  | 2.43                     | 0.51              |
| 1:A:50:SER:HB2    | 1:B:8:PHE:HZ      | 1.76                     | 0.51              |
| 2:C:151:ARG:HH21  | 2:C:156:PHE:HD2   | 1.56                     | 0.51              |
| 2:C:183:TRP:H     | 2:C:199:ASP:HB3   | 1.76                     | 0.51              |
| 3:D:1024:THR:O    | 3:D:1025:MET:HE2  | 2.11                     | 0.51              |
| 2:C:964:LEU:HD21  | 2:C:1025:PHE:HB2  | 1.93                     | 0.51              |
| 2:C:987:GLU:HG3   | 2:C:988:LYS:N     | 2.26                     | 0.51              |
| 2:C:1284:ALA:HB1  | 3:D:1356:LEU:HD22 | 1.92                     | 0.51              |
| 1:A:235:ARG:HE    | 1:B:14:VAL:H      | 1.57                     | 0.51              |
| 3:D:479:GLU:HG2   | 4:E:20:VAL:HG11   | 1.93                     | 0.51              |
| 3:D:1061:VAL:HG21 | 3:D:1101:LEU:HD12 | 1.93                     | 0.51              |
| 5:N:25:DT:H2"     | 5:N:26:DA:C8      | 2.46                     | 0.51              |
| 1:A:155:ALA:O     | 1:A:159:ILE:HG12  | 2.10                     | 0.50              |
| 1:B:133:LEU:HD11  | 1:B:140:ILE:HG22  | 1.92                     | 0.50              |
| 1:A:45:ARG:HD2    | 2:C:1083:GLU:HB2  | 1.93                     | 0.50              |
| 2:C:310:ILE:HD12  | 2:C:325:LEU:HD22  | 1.93                     | 0.50              |
| 3:D:211:GLU:HG3   | 3:D:215:LYS:HZ2   | 1.74                     | 0.50              |
| 3:D:1152:GLU:OE2  | 3:D:1194:ARG:NH2  | 2.44                     | 0.50              |
| 3:D:1344:LEU:C    | 3:D:1346:GLY:H    | 2.14                     | 0.50              |
| 2:C:28:LEU:HD21   | 2:C:524:ILE:HG13  | 1.92                     | 0.50              |
| 2:C:741:MET:SD    | 2:C:746:ALA:HB1   | 2.52                     | 0.50              |
| 3:D:905:ARG:HB3   | 4:E:16:ARG:NH1    | 2.26                     | 0.50              |
| 3:D:1163:VAL:HG23 | 3:D:1177:ILE:HD13 | 1.94                     | 0.50              |
| 1:B:30:PRO:HB2    | 1:B:198:LEU:HD23  | 1.92                     | 0.50              |
| 2:C:406:ASN:HB3   | 2:C:411:ARG:HG3   | 1.93                     | 0.50              |
| 2:C:801:ARG:NH1   | 2:C:1119:MET:HE1  | 2.27                     | 0.50              |
| 3:D:120:LEU:HB2   | 3:D:1330:ARG:NH2  | 2.17                     | 0.50              |
| 1:A:7:GLU:O       | 1:B:150:ARG:NH2   | 2.44                     | 0.50              |
| 5:N:1:DG:H1       | 7:T:29:DC:N4      | 2.09                     | 0.50              |
| 1:A:31:LEU:HD13   | 1:A:36:GLY:HA2    | 1.93                     | 0.50              |
| 2:C:197:ARG:NH1   | 2:C:201:ARG:O     | 2.45                     | 0.50              |
| 2:C:453:ILE:HD11  | 2:C:587:LEU:HG    | 1.92                     | 0.50              |
| 2:C:871:VAL:HG13  | 2:C:883:LEU:O     | 2.11                     | 0.50              |
| 2:C:1072:ASN:ND2  | 2:C:1111:GLN:OE1  | 2.45                     | 0.50              |
| 3:D:113:HIS:CE1   | 3:D:307:LEU:HD13  | 2.46                     | 0.50              |
| 3:D:914:ALA:O     | 3:D:918:ILE:HG13  | 2.12                     | 0.50              |
| 2:C:120:GLN:H     | 2:C:120:GLN:CD    | 2.20                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1122:LYS:HG2  | 2:C:1229:TYR:CZ   | 2.47                     | 0.50              |
| 3:D:253:VAL:HG11  | 6:R:11:C:N3       | 2.26                     | 0.50              |
| 2:C:767:GLN:HA    | 2:C:785:ASP:O     | 2.12                     | 0.50              |
| 2:C:37:LYS:HA     | 2:C:40:GLU:CD     | 2.37                     | 0.50              |
| 2:C:199:ASP:HB2   | 5:N:15:DT:O2      | 2.11                     | 0.50              |
| 2:C:378:ARG:CZ    | 2:C:379:GLU:HG2   | 2.41                     | 0.50              |
| 2:C:538:LEU:H     | 2:C:538:LEU:HD23  | 1.77                     | 0.50              |
| 2:C:1290:MET:CG   | 3:D:347:VAL:HG11  | 2.42                     | 0.50              |
| 3:D:201:LEU:HD11  | 3:D:220:ARG:HD3   | 1.92                     | 0.50              |
| 3:D:378:LYS:NZ    | 3:D:382:TYR:OH    | 2.44                     | 0.50              |
| 3:D:1048:ARG:HH11 | 3:D:1048:ARG:HG2  | 1.77                     | 0.50              |
| 1:A:190:ALA:HB2   | 1:A:200:LYS:HB3   | 1.93                     | 0.49              |
| 2:C:524:ILE:O     | 2:C:528:ARG:HG2   | 2.12                     | 0.49              |
| 2:C:1121:ALA:O    | 2:C:1124:ILE:HG22 | 2.11                     | 0.49              |
| 3:D:535:ARG:HG2   | 3:D:535:ARG:HH11  | 1.77                     | 0.49              |
| 3:D:961:SER:HG    | 3:D:981:GLU:HB3   | 1.77                     | 0.49              |
| 3:D:1052:GLU:OE1  | 3:D:1052:GLU:N    | 2.39                     | 0.49              |
| 7:T:20:DC:H2'     | 7:T:21:DT:C6      | 2.47                     | 0.49              |
| 1:B:33:ARG:HD3    | 1:B:197:ASP:HB2   | 1.94                     | 0.49              |
| 2:C:71:VAL:HG21   | 2:C:118:LYS:HE3   | 1.93                     | 0.49              |
| 2:C:690:VAL:HG22  | 2:C:1234:LYS:O    | 2.12                     | 0.49              |
| 2:C:958:LYS:O     | 2:C:962:GLU:HG3   | 2.12                     | 0.49              |
| 3:D:357:VAL:HG23  | 3:D:358:GLY:N     | 2.24                     | 0.49              |
| 2:C:26:TYR:CE2    | 2:C:28:LEU:HB2    | 2.47                     | 0.49              |
| 2:C:517:GLN:H     | 2:C:761:GLN:HE21  | 1.59                     | 0.49              |
| 3:D:85:CYS:HB3    | 3:D:88:CYS:O      | 2.11                     | 0.49              |
| 1:B:32:GLU:HB3    | 1:B:35:PHE:CD1    | 2.47                     | 0.49              |
| 2:C:128:PRO:HG2   | 2:C:506:PHE:HD2   | 1.76                     | 0.49              |
| 2:C:371:ARG:HA    | 2:C:371:ARG:HH11  | 1.78                     | 0.49              |
| 2:C:681:MET:O     | 2:C:685:MET:HE2   | 2.12                     | 0.49              |
| 3:D:977:SER:HB2   | 3:D:980:THR:HG23  | 1.94                     | 0.49              |
| 3:D:1150:PRO:C    | 3:D:1152:GLU:H    | 2.20                     | 0.49              |
| 1:A:9:LEU:O       | 1:A:10:LYS:HG3    | 2.12                     | 0.49              |
| 3:D:1267:VAL:O    | 3:D:1274:PHE:HE1  | 1.94                     | 0.49              |
| 1:A:57:THR:HB     | 1:A:158:ARG:HH12  | 1.77                     | 0.49              |
| 2:C:49:LEU:HD23   | 2:C:73:TYR:CE2    | 2.47                     | 0.49              |
| 3:D:793:SER:HB2   | 3:D:1138:LEU:HD21 | 1.93                     | 0.49              |
| 1:B:166:ARG:NE    | 1:B:167:PRO:HD2   | 2.28                     | 0.49              |
| 2:C:21:VAL:HG11   | 2:C:592:ARG:HD2   | 1.94                     | 0.49              |
| 2:C:94:ALA:HB2    | 2:C:129:LEU:HD11  | 1.94                     | 0.49              |
| 2:C:588:GLU:HG2   | 2:C:607:SER:N     | 2.27                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1276:TRP:CD2  | 3:D:801:VAL:HG11  | 2.48                     | 0.49              |
| 3:D:44:ILE:HD12   | 3:D:252:LEU:HD22  | 1.95                     | 0.49              |
| 3:D:201:LEU:O     | 3:D:205:LEU:HD23  | 2.12                     | 0.49              |
| 3:D:1075:ARG:HG2  | 3:D:1100:PHE:HE2  | 1.76                     | 0.49              |
| 2:C:62:TYR:CE2    | 2:C:476:LYS:HG3   | 2.47                     | 0.49              |
| 2:C:1106:ARG:O    | 2:C:1108:ASN:N    | 2.40                     | 0.49              |
| 2:C:1212:LEU:HD12 | 2:C:1225:VAL:HG21 | 1.95                     | 0.49              |
| 3:D:102:MET:HE2   | 3:D:243:PRO:HB2   | 1.94                     | 0.49              |
| 3:D:1227:HIS:HA   | 3:D:1230:THR:HG22 | 1.95                     | 0.49              |
| 2:C:742:TYR:O     | 2:C:746:ALA:HB2   | 2.13                     | 0.49              |
| 3:D:1021:ASP:HB3  | 3:D:1024:THR:HB   | 1.94                     | 0.49              |
| 2:C:1290:MET:HG2  | 3:D:347:VAL:HG11  | 1.94                     | 0.49              |
| 3:D:580:TRP:CZ3   | 3:D:589:TYR:HA    | 2.48                     | 0.49              |
| 1:B:62:ASP:OD2    | 1:B:141:SER:HB3   | 2.12                     | 0.48              |
| 2:C:1033:ARG:HA   | 2:C:1036:ILE:HG22 | 1.95                     | 0.48              |
| 3:D:337:ARG:O     | 3:D:338:PHE:C     | 2.55                     | 0.48              |
| 3:D:555:TYR:CD2   | 3:D:585:LYS:HD2   | 2.48                     | 0.48              |
| 3:D:959:LYS:HA    | 3:D:959:LYS:HE2   | 1.93                     | 0.48              |
| 2:C:813:GLU:C     | 2:C:815:SER:H     | 2.21                     | 0.48              |
| 2:C:1264:GLN:O    | 2:C:1265:PHE:C    | 2.56                     | 0.48              |
| 3:D:369:PRO:HB3   | 3:D:444:GLY:O     | 2.13                     | 0.48              |
| 3:D:638:SER:OG    | 3:D:639:VAL:N     | 2.46                     | 0.48              |
| 3:D:644:MET:HG3   | 3:D:764:ARG:HD2   | 1.94                     | 0.48              |
| 3:D:975:ILE:HG23  | 3:D:980:THR:HG21  | 1.95                     | 0.48              |
| 2:C:96:LEU:C      | 2:C:97:ARG:HD2    | 2.39                     | 0.48              |
| 2:C:194:LEU:H     | 2:C:350:THR:CG2   | 2.27                     | 0.48              |
| 2:C:1112:ILE:HD11 | 3:D:639:VAL:HG23  | 1.96                     | 0.48              |
| 1:A:218:ARG:NH1   | 1:B:231:PHE:HA    | 2.27                     | 0.48              |
| 2:C:551:HIS:ND1   | 2:C:552:PRO:HD2   | 2.28                     | 0.48              |
| 2:C:561:ILE:HD11  | 2:C:665:ALA:HB1   | 1.96                     | 0.48              |
| 3:D:149:GLY:O     | 3:D:152:THR:HG22  | 2.13                     | 0.48              |
| 1:B:133:LEU:HD21  | 1:B:140:ILE:HB    | 1.95                     | 0.48              |
| 2:C:683:ALA:O     | 2:C:687:ARG:HG3   | 2.13                     | 0.48              |
| 3:D:527:LEU:HB2   | 3:D:550:VAL:HG22  | 1.95                     | 0.48              |
| 3:D:821:MET:SD    | 3:D:879:ALA:HB1   | 2.53                     | 0.48              |
| 7:T:20:DC:H2'     | 7:T:21:DT:H71     | 1.96                     | 0.48              |
| 1:A:208:ASN:OD1   | 1:A:210:THR:HG22  | 2.13                     | 0.48              |
| 1:B:192:VAL:C     | 1:B:194:GLN:H     | 2.21                     | 0.48              |
| 2:C:452:ARG:NH1   | 2:C:458:GLU:OE2   | 2.44                     | 0.48              |
| 3:D:709:ARG:HG3   | 3:D:710:ASP:H     | 1.78                     | 0.48              |
| 2:C:16:GLY:HA2    | 2:C:1188:ASP:OD1  | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:228:VAL:HB    | 2:C:335:THR:CG2   | 2.43                     | 0.48              |
| 2:C:1122:LYS:HG2  | 2:C:1229:TYR:CE1  | 2.49                     | 0.48              |
| 3:D:244:VAL:HG12  | 3:D:269:TYR:CE1   | 2.48                     | 0.48              |
| 2:C:514:PHE:HE2   | 7:T:20:DC:H4'     | 1.78                     | 0.48              |
| 2:C:541:GLU:HG2   | 2:C:542:ARG:N     | 2.28                     | 0.48              |
| 3:D:356:THR:HG22  | 3:D:357:VAL:H     | 1.77                     | 0.48              |
| 3:D:901:ARG:HD2   | 3:D:906:GLY:O     | 2.14                     | 0.48              |
| 1:A:215:GLU:OE1   | 1:A:215:GLU:N     | 2.47                     | 0.48              |
| 2:C:919:ARG:HG3   | 2:C:919:ARG:HH11  | 1.78                     | 0.48              |
| 2:C:1254:VAL:HG13 | 2:C:1255:THR:H    | 1.78                     | 0.48              |
| 3:D:130:MET:HE2   | 3:D:157:GLN:HB3   | 1.95                     | 0.48              |
| 3:D:369:PRO:HG2   | 3:D:372:MET:HE3   | 1.96                     | 0.48              |
| 4:E:68:GLU:OE2    | 4:E:69:ARG:HG3    | 2.13                     | 0.48              |
| 1:A:158:ARG:HH22  | 1:A:175:ALA:HB2   | 1.79                     | 0.47              |
| 3:D:1194:ARG:HD2  | 3:D:1211:SER:CB   | 2.43                     | 0.47              |
| 2:C:253:PHE:HA    | 2:C:265:LYS:HD2   | 1.95                     | 0.47              |
| 2:C:696:ASP:O     | 2:C:697:LYS:HB3   | 2.12                     | 0.47              |
| 2:C:1158:LYS:HE2  | 2:C:1158:LYS:HB2  | 1.53                     | 0.47              |
| 1:A:61:ILE:HB     | 1:A:64:VAL:CG2    | 2.45                     | 0.47              |
| 1:B:79:LEU:HD23   | 3:D:526:VAL:HG11  | 1.96                     | 0.47              |
| 2:C:10:ARG:NH1    | 2:C:697:LYS:HD3   | 2.29                     | 0.47              |
| 2:C:395:TYR:CE2   | 2:C:420:LEU:HG    | 2.49                     | 0.47              |
| 2:C:636:CYS:O     | 2:C:642:SER:HA    | 2.14                     | 0.47              |
| 2:C:97:ARG:HG2    | 2:C:121:GLU:OE1   | 2.14                     | 0.47              |
| 2:C:1298:VAL:HG23 | 2:C:1299:ASN:N    | 2.30                     | 0.47              |
| 3:D:167:ASP:HA    | 3:D:170:GLU:OE2   | 2.14                     | 0.47              |
| 3:D:607:THR:HA    | 3:D:610:ARG:HG2   | 1.96                     | 0.47              |
| 2:C:255:ILE:HD13  | 2:C:263:VAL:HB    | 1.97                     | 0.47              |
| 2:C:1021:LEU:O    | 2:C:1024:GLU:HG3  | 2.14                     | 0.47              |
| 2:C:1293:VAL:HG21 | 2:C:1315:MET:HG3  | 1.96                     | 0.47              |
| 3:D:438:GLU:CD    | 4:E:2:ALA:CB      | 2.80                     | 0.47              |
| 3:D:1162:ILE:HD13 | 3:D:1203:ARG:HH22 | 1.78                     | 0.47              |
| 1:A:154:PRO:HG2   | 1:A:157:THR:HG23  | 1.96                     | 0.47              |
| 2:C:120:GLN:OE1   | 2:C:120:GLN:N     | 2.40                     | 0.47              |
| 2:C:305:SER:OG    | 2:C:306:THR:N     | 2.48                     | 0.47              |
| 2:C:835:GLU:C     | 2:C:836:LEU:HD12  | 2.39                     | 0.47              |
| 3:D:615:LYS:CE    | 4:E:5:THR:HB      | 2.44                     | 0.47              |
| 4:E:7:GLN:O       | 4:E:10:VAL:HG12   | 2.14                     | 0.47              |
| 2:C:213:LEU:HD12  | 2:C:422:LYS:HB3   | 1.95                     | 0.47              |
| 2:C:864:LYS:NZ    | 2:C:881:ASP:HB3   | 2.29                     | 0.47              |
| 3:D:53:ARG:HA     | 3:D:53:ARG:HD3    | 1.43                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:163:GLU:HA    | 3:D:166:LEU:HD12  | 1.96                     | 0.47              |
| 3:D:338:PHE:HA    | 3:D:342:LEU:HB2   | 1.96                     | 0.47              |
| 3:D:733:SER:N     | 3:D:736:GLN:OE1   | 2.38                     | 0.47              |
| 3:D:1110:GLU:HG2  | 3:D:1111:ASP:N    | 2.29                     | 0.47              |
| 3:D:1342:ASP:OD2  | 3:D:1344:LEU:HD23 | 2.14                     | 0.47              |
| 4:E:28:ARG:O      | 4:E:32:VAL:HG22   | 2.14                     | 0.47              |
| 1:B:102:LEU:HD21  | 1:B:110:VAL:HG11  | 1.97                     | 0.47              |
| 1:B:223:ILE:HA    | 1:B:226:GLU:OE1   | 2.15                     | 0.47              |
| 2:C:754:THR:HG22  | 2:C:767:GLN:NE2   | 2.29                     | 0.47              |
| 2:C:820:GLU:O     | 2:C:824:GLN:HG3   | 2.15                     | 0.47              |
| 2:C:1275:VAL:O    | 2:C:1279:GLU:HG3  | 2.14                     | 0.47              |
| 3:D:204:GLU:OE1   | 3:D:205:LEU:HD22  | 2.15                     | 0.47              |
| 3:D:279:LEU:HD11  | 3:D:296:LYS:HG2   | 1.95                     | 0.47              |
| 3:D:666:GLU:O     | 3:D:669:GLN:HG2   | 2.15                     | 0.47              |
| 3:D:861:ASN:O     | 3:D:861:ASN:ND2   | 2.28                     | 0.47              |
| 3:D:963:VAL:HB    | 3:D:980:THR:HG22  | 1.96                     | 0.47              |
| 1:A:45:ARG:HE     | 2:C:1083:GLU:HG3  | 1.80                     | 0.47              |
| 1:B:75:GLN:HG2    | 1:B:76:GLU:N      | 2.27                     | 0.47              |
| 2:C:1298:VAL:HG13 | 2:C:1321:GLU:HG3  | 1.97                     | 0.47              |
| 3:D:221:ILE:O     | 3:D:225:GLU:HG3   | 2.15                     | 0.47              |
| 3:D:847:ASP:HB2   | 3:D:856:ILE:HG23  | 1.96                     | 0.47              |
| 2:C:397:LEU:O     | 2:C:398:SER:OG    | 2.24                     | 0.47              |
| 2:C:570:GLY:HA2   | 3:D:780:ARG:HH12  | 1.79                     | 0.47              |
| 2:C:1255:THR:O    | 2:C:1257:GLN:N    | 2.42                     | 0.47              |
| 3:D:26:SER:HB2    | 3:D:236:TRP:CZ2   | 2.50                     | 0.47              |
| 3:D:88:CYS:C      | 3:D:90:VAL:H      | 2.23                     | 0.47              |
| 2:C:122:VAL:HG21  | 2:C:493:ILE:HG21  | 1.96                     | 0.46              |
| 2:C:755:LYS:NZ    | 2:C:767:GLN:O     | 2.39                     | 0.46              |
| 2:C:820:GLU:N     | 2:C:1080:ASN:O    | 2.38                     | 0.46              |
| 3:D:505:ASP:HB2   | 3:D:629:PHE:HE1   | 1.80                     | 0.46              |
| 3:D:804:ALA:HA    | 3:D:1259:GLN:HG3  | 1.97                     | 0.46              |
| 3:D:913:GLU:OE2   | 4:E:17:PHE:CZ     | 2.68                     | 0.46              |
| 1:A:82:LEU:HD21   | 1:A:171:LEU:HB3   | 1.97                     | 0.46              |
| 1:B:80:GLU:OE2    | 3:D:569:LEU:HD13  | 2.16                     | 0.46              |
| 2:C:88:ARG:HH11   | 2:C:88:ARG:CB     | 2.27                     | 0.46              |
| 2:C:131:THR:HG22  | 2:C:132:ASP:N     | 2.29                     | 0.46              |
| 2:C:577:VAL:HG23  | 2:C:661:VAL:O     | 2.15                     | 0.46              |
| 2:C:866:ASP:HB3   | 2:C:872:TYR:CE1   | 2.50                     | 0.46              |
| 2:C:994:ARG:HA    | 2:C:997:TRP:NE1   | 2.29                     | 0.46              |
| 2:C:1283:ALA:HA   | 3:D:479:GLU:OE1   | 2.15                     | 0.46              |
| 1:A:98:VAL:HG11   | 1:A:121:VAL:HG21  | 1.97                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:120:ASP:OD1  | 1:A:121:VAL:HG23  | 2.15                     | 0.46              |
| 2:C:46:GLN:NE2   | 2:C:47:TYR:HB2    | 2.29                     | 0.46              |
| 3:D:38:VAL:HG23  | 3:D:105:ILE:HG12  | 1.96                     | 0.46              |
| 3:D:45:ASN:O     | 3:D:47:ARG:N      | 2.47                     | 0.46              |
| 3:D:458:ASN:HD22 | 3:D:929:GLN:NE2   | 2.14                     | 0.46              |
| 3:D:1346:GLY:HA3 | 3:D:1349:GLU:OE2  | 2.16                     | 0.46              |
| 1:A:233:ASP:OD1  | 1:A:234:LEU:N     | 2.49                     | 0.46              |
| 2:C:58:PRO:HB3   | 2:C:67:GLU:OE2    | 2.16                     | 0.46              |
| 3:D:574:VAL:O    | 3:D:578:ILE:HG12  | 2.15                     | 0.46              |
| 3:D:972:LYS:HZ3  | 3:D:974:VAL:HA    | 1.81                     | 0.46              |
| 2:C:615:VAL:HG23 | 2:C:650:VAL:HA    | 1.96                     | 0.46              |
| 3:D:614:LEU:HD23 | 4:E:5:THR:HG21    | 1.96                     | 0.46              |
| 3:D:1344:LEU:HA  | 3:D:1349:GLU:HG3  | 1.98                     | 0.46              |
| 1:B:46:ILE:HD11  | 1:B:224:LEU:HD13  | 1.98                     | 0.46              |
| 2:C:12:ARG:HD3   | 2:C:1183:ALA:HB2  | 1.96                     | 0.46              |
| 2:C:41:GLN:HA    | 2:C:41:GLN:OE1    | 2.16                     | 0.46              |
| 2:C:175:ARG:HG3  | 2:C:185:ASP:OD1   | 2.16                     | 0.46              |
| 3:D:42:GLU:HB3   | 3:D:52:GLU:HG2    | 1.96                     | 0.46              |
| 2:C:631:GLU:O    | 2:C:647:ARG:HD3   | 2.14                     | 0.46              |
| 2:C:883:LEU:HD21 | 2:C:920:VAL:HG22  | 1.97                     | 0.46              |
| 2:C:1136:GLN:HB3 | 2:C:1140:LYS:HD2  | 1.97                     | 0.46              |
| 3:D:836:ARG:HB2  | 3:D:873:GLU:OE2   | 2.15                     | 0.46              |
| 2:C:39:ILE:O     | 2:C:73:TYR:OH     | 2.34                     | 0.46              |
| 2:C:88:ARG:HB2   | 2:C:88:ARG:HH11   | 1.80                     | 0.46              |
| 2:C:178:PRO:HG3  | 2:C:395:TYR:CE1   | 2.51                     | 0.46              |
| 3:D:698:MET:O    | 3:D:702:GLN:HB2   | 2.16                     | 0.46              |
| 3:D:557:LYS:HB3  | 3:D:563:LEU:HD23  | 1.97                     | 0.46              |
| 3:D:596:LEU:HD23 | 3:D:596:LEU:HA    | 1.74                     | 0.46              |
| 1:B:212:ASP:OD1  | 1:B:212:ASP:N     | 2.49                     | 0.46              |
| 2:C:1033:ARG:O   | 2:C:1036:ILE:HG22 | 2.16                     | 0.46              |
| 2:C:1298:VAL:HA  | 2:C:1301:ARG:NH2  | 2.31                     | 0.46              |
| 4:E:65:ASP:O     | 4:E:68:GLU:HG3    | 2.15                     | 0.46              |
| 1:A:166:ARG:HD3  | 1:A:166:ARG:N     | 2.30                     | 0.45              |
| 1:B:156:SER:HA   | 1:B:159:ILE:HG22  | 1.98                     | 0.45              |
| 7:T:12:DG:H2'    | 7:T:13:DT:C6      | 2.51                     | 0.45              |
| 2:C:48:GLY:O     | 2:C:51:ALA:N      | 2.45                     | 0.45              |
| 3:D:57:PHE:CD2   | 3:D:247:PRO:HB3   | 2.50                     | 0.45              |
| 3:D:297:ARG:O    | 3:D:301:GLU:OE1   | 2.34                     | 0.45              |
| 3:D:511:TYR:CZ   | 3:D:515:ARG:HD2   | 2.51                     | 0.45              |
| 4:E:32:VAL:O     | 4:E:34:GLY:N      | 2.43                     | 0.45              |
| 4:E:50:ALA:O     | 4:E:54:ILE:HG12   | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:528:ARG:NH1   | 2:C:576:SER:O     | 2.49                     | 0.45              |
| 3:D:139:LEU:HD21  | 3:D:300:GLN:HG2   | 1.97                     | 0.45              |
| 3:D:955:LYS:CE    | 3:D:1012:ALA:HA   | 2.46                     | 0.45              |
| 1:B:193:GLU:HG2   | 1:B:194:GLN:HG2   | 1.98                     | 0.45              |
| 2:C:756:TYR:HD1   | 2:C:764:CYS:SG    | 2.39                     | 0.45              |
| 2:C:818:VAL:HG21  | 2:C:1076:ILE:HD12 | 1.99                     | 0.45              |
| 3:D:630:ALA:O     | 3:D:634:ARG:HG3   | 2.16                     | 0.45              |
| 3:D:1044:GLN:OE1  | 3:D:1044:GLN:N    | 2.49                     | 0.45              |
| 3:D:1156:LEU:HD21 | 3:D:1224:ARG:HH21 | 1.81                     | 0.45              |
| 1:B:56:VAL:HG12   | 1:B:146:VAL:HG12  | 1.98                     | 0.45              |
| 2:C:31:GLN:O      | 2:C:130:MET:HE1   | 2.16                     | 0.45              |
| 2:C:241:LEU:HD11  | 2:C:246:LEU:CD2   | 2.47                     | 0.45              |
| 2:C:1254:VAL:HG13 | 2:C:1255:THR:N    | 2.32                     | 0.45              |
| 1:B:47:LEU:HD23   | 1:B:51:MET:SD     | 2.56                     | 0.45              |
| 2:C:155:VAL:O     | 2:C:156:PHE:HD1   | 2.00                     | 0.45              |
| 2:C:559:CYS:HB2   | 2:C:662:SER:HB2   | 1.98                     | 0.45              |
| 2:C:588:GLU:HG2   | 2:C:607:SER:CA    | 2.47                     | 0.45              |
| 2:C:699:LEU:HG    | 2:C:799:ASN:ND2   | 2.32                     | 0.45              |
| 2:C:850:ILE:HG22  | 2:C:850:ILE:O     | 2.16                     | 0.45              |
| 2:C:1274:GLU:HG2  | 3:D:424:ASN:ND2   | 2.31                     | 0.45              |
| 3:D:464:ASP:OD1   | 6:R:20:A:O2'      | 2.18                     | 0.45              |
| 2:C:465:ARG:HG3   | 2:C:465:ARG:HH11  | 1.82                     | 0.45              |
| 2:C:996:ARG:C     | 2:C:997:TRP:HD1   | 2.25                     | 0.45              |
| 4:E:18:ASP:O      | 4:E:22:VAL:HG12   | 2.17                     | 0.45              |
| 4:E:36:ASP:OD1    | 4:E:37:PRO:HD2    | 2.16                     | 0.45              |
| 5:N:20:DG:H1'     | 5:N:21:DC:H5'     | 1.98                     | 0.45              |
| 1:B:54:CYS:SG     | 1:B:92:VAL:HG22   | 2.56                     | 0.45              |
| 1:B:134:THR:HG22  | 1:B:135:ASP:N     | 2.27                     | 0.45              |
| 2:C:334:GLU:OE1   | 2:C:334:GLU:HA    | 2.17                     | 0.45              |
| 2:C:499:SER:HA    | 2:C:502:VAL:HG12  | 1.98                     | 0.45              |
| 2:C:1124:ILE:HD11 | 2:C:1148:ALA:CB   | 2.47                     | 0.45              |
| 2:C:1134:GLN:O    | 2:C:1135:GLN:HG2  | 2.17                     | 0.45              |
| 3:D:131:PRO:HG2   | 3:D:134:ASP:OD2   | 2.17                     | 0.45              |
| 3:D:314:ARG:NH1   | 3:D:314:ARG:HB3   | 2.32                     | 0.45              |
| 3:D:450:HIS:O     | 3:D:453:VAL:HG22  | 2.17                     | 0.45              |
| 3:D:1232:TYR:O    | 3:D:1236:GLU:HG2  | 2.17                     | 0.45              |
| 2:C:150:HIS:NE2   | 2:C:454:ARG:HG3   | 2.32                     | 0.45              |
| 2:C:576:SER:OG    | 2:C:659:GLN:O     | 2.33                     | 0.45              |
| 3:D:115:TRP:CZ2   | 3:D:1329:THR:HG22 | 2.52                     | 0.45              |
| 3:D:116:PHE:CD1   | 3:D:1333:THR:HG23 | 2.51                     | 0.45              |
| 3:D:587:LEU:HD11  | 3:D:608:CYS:HB2   | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1033:GLY:HA3  | 3:D:1082:ASP:HA   | 1.98                     | 0.45              |
| 3:D:1194:ARG:HA   | 3:D:1194:ARG:NE   | 2.32                     | 0.45              |
| 3:D:1311:LYS:HD3  | 3:D:1311:LYS:HA   | 1.70                     | 0.45              |
| 2:C:213:LEU:O     | 2:C:214:ASN:HB3   | 2.17                     | 0.45              |
| 2:C:275:ARG:O     | 2:C:279:LYS:HG2   | 2.17                     | 0.45              |
| 2:C:321:LEU:O     | 2:C:325:LEU:HD23  | 2.16                     | 0.45              |
| 3:D:167:ASP:O     | 3:D:171:GLU:HG3   | 2.17                     | 0.45              |
| 3:D:357:VAL:HG12  | 3:D:461:PHE:CD2   | 2.52                     | 0.45              |
| 3:D:661:VAL:HA    | 3:D:664:ILE:HG22  | 1.98                     | 0.45              |
| 2:C:301:TYR:HB3   | 2:C:330:HIS:CE1   | 2.52                     | 0.44              |
| 3:D:60:ARG:HD3    | 3:D:89:GLY:CA     | 2.47                     | 0.44              |
| 3:D:1280:VAL:HG21 | 3:D:1304:ARG:HD2  | 1.98                     | 0.44              |
| 1:B:222:THR:O     | 1:B:226:GLU:OE1   | 2.35                     | 0.44              |
| 2:C:407:ARG:HH21  | 2:C:414:ILE:HD12  | 1.83                     | 0.44              |
| 2:C:456:VAL:HG13  | 2:C:457:GLY:N     | 2.32                     | 0.44              |
| 2:C:591:TYR:CE1   | 2:C:616:ILE:HG21  | 2.52                     | 0.44              |
| 2:C:843:THR:OG1   | 2:C:846:GLY:O     | 2.36                     | 0.44              |
| 2:C:964:LEU:HD11  | 2:C:1025:PHE:CD1  | 2.52                     | 0.44              |
| 2:C:1270:PHE:CE1  | 2:C:1274:GLU:HB3  | 2.53                     | 0.44              |
| 3:D:202:ARG:NH2   | 3:D:225:GLU:OE2   | 2.41                     | 0.44              |
| 3:D:518:VAL:HG22  | 3:D:707:ILE:HD11  | 1.99                     | 0.44              |
| 3:D:741:ALA:C     | 3:D:762:ASN:HD22  | 2.24                     | 0.44              |
| 3:D:1040:MET:SD   | 3:D:1046:ILE:HG13 | 2.57                     | 0.44              |
| 4:E:15:ASN:HB3    | 4:E:18:ASP:OD1    | 2.16                     | 0.44              |
| 2:C:197:ARG:NH2   | 2:C:203:LYS:HB3   | 2.32                     | 0.44              |
| 2:C:817:LEU:HD23  | 2:C:1097:VAL:HB   | 1.98                     | 0.44              |
| 2:C:937:ASP:OD1   | 2:C:1047:LEU:HB3  | 2.17                     | 0.44              |
| 2:C:1244:HIS:CE1  | 2:C:1265:PHE:O    | 2.71                     | 0.44              |
| 3:D:144:TYR:N     | 3:D:160:LEU:O     | 2.49                     | 0.44              |
| 3:D:148:GLU:OE2   | 3:D:156:ARG:HD2   | 2.17                     | 0.44              |
| 3:D:643:ASP:O     | 3:D:720:ASN:ND2   | 2.34                     | 0.44              |
| 3:D:843:VAL:HG23  | 3:D:883:ARG:HD3   | 1.98                     | 0.44              |
| 3:D:1175:LEU:HB2  | 3:D:1190:ILE:HD11 | 2.00                     | 0.44              |
| 3:D:1329:THR:O    | 3:D:1333:THR:OG1  | 2.26                     | 0.44              |
| 2:C:257:ALA:HB3   | 2:C:262:TYR:HE2   | 1.82                     | 0.44              |
| 2:C:615:VAL:HG12  | 2:C:638:SER:HB3   | 2.00                     | 0.44              |
| 3:D:424:ASN:HB2   | 3:D:434:ILE:HG12  | 1.99                     | 0.44              |
| 3:D:537:TYR:CE1   | 3:D:544:LEU:HB2   | 2.52                     | 0.44              |
| 3:D:759:ILE:HG23  | 3:D:771:GLN:HB3   | 1.99                     | 0.44              |
| 2:C:540:ARG:HG3   | 2:C:541:GLU:N     | 2.32                     | 0.44              |
| 2:C:595:THR:O     | 2:C:597:GLY:N     | 2.50                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1270:PHE:CZ   | 2:C:1274:GLU:HB3  | 2.53                     | 0.44              |
| 3:D:60:ARG:NE     | 3:D:89:GLY:H      | 2.15                     | 0.44              |
| 3:D:510:LEU:HD21  | 3:D:579:LEU:HD13  | 2.00                     | 0.44              |
| 3:D:886:VAL:HG11  | 3:D:1230:THR:HG21 | 2.00                     | 0.44              |
| 3:D:1035:VAL:HG23 | 3:D:1078:LEU:HG   | 1.98                     | 0.44              |
| 3:D:1146:GLU:O    | 3:D:1146:GLU:HG3  | 2.18                     | 0.44              |
| 1:B:167:PRO:HB2   | 1:B:170:ARG:NH2   | 2.23                     | 0.44              |
| 2:C:107:ARG:HD2   | 2:C:107:ARG:HA    | 1.69                     | 0.44              |
| 2:C:544:GLY:O     | 2:C:547:VAL:HG12  | 2.18                     | 0.44              |
| 2:C:564:PRO:HD2   | 2:C:572:ILE:HB    | 2.00                     | 0.44              |
| 2:C:755:LYS:O     | 2:C:756:TYR:C     | 2.60                     | 0.44              |
| 2:C:800:MET:CE    | 2:C:828:PHE:HE2   | 2.31                     | 0.44              |
| 2:C:1023:HIS:CD2  | 2:C:1027:LYS:NZ   | 2.86                     | 0.44              |
| 2:C:1253:LEU:HD13 | 6:R:11:C:H1'      | 2.00                     | 0.44              |
| 3:D:557:LYS:HA    | 3:D:562:GLU:O     | 2.17                     | 0.44              |
| 3:D:1059:LEU:HB2  | 3:D:1107:VAL:HB   | 2.00                     | 0.44              |
| 3:D:1197:ASN:OD1  | 3:D:1198:VAL:HG13 | 2.16                     | 0.44              |
| 2:C:488:MET:SD    | 2:C:489:PRO:HD2   | 2.57                     | 0.44              |
| 2:C:886:LYS:H     | 2:C:917:SER:HG    | 1.59                     | 0.44              |
| 2:C:1230:MET:HG2  | 2:C:1231:TYR:N    | 2.32                     | 0.44              |
| 3:D:94:GLN:O      | 3:D:97:VAL:HG12   | 2.18                     | 0.44              |
| 3:D:155:GLU:OE2   | 3:D:158:GLN:HB2   | 2.17                     | 0.44              |
| 3:D:475:GLU:O     | 3:D:479:GLU:HG3   | 2.18                     | 0.44              |
| 3:D:661:VAL:HG22  | 3:D:685:ILE:HD11  | 2.00                     | 0.44              |
| 3:D:831:VAL:HG23  | 3:D:831:VAL:O     | 2.17                     | 0.44              |
| 3:D:836:ARG:CG    | 3:D:869:CYS:HB3   | 2.47                     | 0.44              |
| 7:T:15:DT:H2'     | 7:T:16:DA:C8      | 2.53                     | 0.44              |
| 1:B:140:ILE:HD11  | 1:B:142:MET:HE3   | 2.00                     | 0.44              |
| 2:C:163:LYS:HD2   | 5:N:19:DG:OP1     | 2.18                     | 0.44              |
| 2:C:224:PHE:HD2   | 2:C:347:ILE:HG21  | 1.83                     | 0.44              |
| 2:C:794:LEU:HD12  | 2:C:794:LEU:HA    | 1.79                     | 0.44              |
| 2:C:810:TYR:HA    | 3:D:357:VAL:HG21  | 2.00                     | 0.44              |
| 2:C:1098:LEU:HD12 | 2:C:1098:LEU:HA   | 1.85                     | 0.44              |
| 3:D:40:LYS:HE2    | 3:D:42:GLU:HB3    | 1.99                     | 0.44              |
| 3:D:56:LEU:HD23   | 3:D:56:LEU:HA     | 1.78                     | 0.44              |
| 1:B:142:MET:SD    | 1:B:144:ILE:HD11  | 2.57                     | 0.44              |
| 2:C:591:TYR:OH    | 2:C:637:ARG:NH2   | 2.51                     | 0.44              |
| 2:C:726:TYR:HB3   | 2:C:733:VAL:HB    | 2.00                     | 0.44              |
| 2:C:1293:VAL:O    | 2:C:1301:ARG:HG2  | 2.18                     | 0.44              |
| 3:D:319:SER:HB3   | 7:T:25:DA:H5''    | 1.99                     | 0.44              |
| 3:D:352:ARG:HE    | 3:D:465:GLN:HE21  | 1.66                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:968:ASN:ND2   | 3:D:1030:GLU:O    | 2.24                     | 0.44              |
| 2:C:153:PRO:HB2   | 2:C:401:GLY:CA    | 2.48                     | 0.43              |
| 2:C:817:LEU:HD11  | 2:C:1080:ASN:ND2  | 2.33                     | 0.43              |
| 3:D:252:LEU:O     | 3:D:252:LEU:HD23  | 2.18                     | 0.43              |
| 3:D:607:THR:HG22  | 3:D:610:ARG:NH1   | 2.33                     | 0.43              |
| 3:D:747:MET:HB2   | 3:D:755:ILE:HD13  | 2.00                     | 0.43              |
| 3:D:849:LEU:HD23  | 3:D:854:ALA:H     | 1.83                     | 0.43              |
| 1:A:73:GLY:O      | 1:A:134:THR:N     | 2.50                     | 0.43              |
| 2:C:61:SER:O      | 2:C:63:SER:N      | 2.51                     | 0.43              |
| 2:C:344:GLY:HA2   | 2:C:345:PRO:HD3   | 1.80                     | 0.43              |
| 2:C:506:PHE:O     | 2:C:512:SER:OG    | 2.24                     | 0.43              |
| 2:C:556:GLY:HA2   | 2:C:659:GLN:O     | 2.18                     | 0.43              |
| 2:C:871:VAL:HG21  | 2:C:928:VAL:HG21  | 1.99                     | 0.43              |
| 3:D:644:MET:SD    | 3:D:764:ARG:HB2   | 2.58                     | 0.43              |
| 3:D:811:GLU:OE2   | 3:D:814:CYS:HA    | 2.17                     | 0.43              |
| 3:D:834:PRO:HD2   | 3:D:837:ASP:OD2   | 2.18                     | 0.43              |
| 1:A:162:GLU:HG2   | 1:A:163:GLU:N     | 2.32                     | 0.43              |
| 2:C:395:TYR:HE2   | 2:C:420:LEU:HG    | 1.84                     | 0.43              |
| 2:C:985:GLU:OE2   | 2:C:988:LYS:N     | 2.50                     | 0.43              |
| 2:C:1124:ILE:HD11 | 2:C:1148:ALA:HB1  | 2.00                     | 0.43              |
| 2:C:1289:GLU:HG3  | 2:C:1290:MET:N    | 2.33                     | 0.43              |
| 3:D:146:VAL:CG2   | 3:D:158:GLN:HB3   | 2.48                     | 0.43              |
| 3:D:331:ILE:HG22  | 3:D:1328:THR:HG21 | 1.99                     | 0.43              |
| 3:D:413:ASP:O     | 3:D:416:ILE:HG22  | 2.18                     | 0.43              |
| 2:C:800:MET:HE3   | 2:C:800:MET:HB2   | 1.85                     | 0.43              |
| 2:C:813:GLU:HB3   | 3:D:460:ASP:OD1   | 2.17                     | 0.43              |
| 2:C:1243:MET:CG   | 3:D:372:MET:HE2   | 2.48                     | 0.43              |
| 3:D:304:ASP:OD1   | 3:D:305:ALA:N     | 2.51                     | 0.43              |
| 3:D:756:GLU:O     | 3:D:758:PRO:HD2   | 2.19                     | 0.43              |
| 3:D:986:ASP:OD1   | 3:D:987:GLU:N     | 2.49                     | 0.43              |
| 2:C:119:GLU:OE1   | 2:C:489:PRO:HD2   | 2.19                     | 0.43              |
| 2:C:575:LEU:HD23  | 2:C:576:SER:N     | 2.34                     | 0.43              |
| 2:C:611:GLU:HG3   | 2:C:616:ILE:HD12  | 1.98                     | 0.43              |
| 2:C:719:LYS:O     | 2:C:779:ARG:HG3   | 2.19                     | 0.43              |
| 2:C:1332:SER:O    | 3:D:243:PRO:HG2   | 2.18                     | 0.43              |
| 3:D:186:GLN:O     | 3:D:190:LYS:HG3   | 2.19                     | 0.43              |
| 3:D:913:GLU:CD    | 4:E:17:PHE:CZ     | 2.95                     | 0.43              |
| 3:D:1062:LEU:HD12 | 3:D:1066:GLU:HG3  | 2.01                     | 0.43              |
| 3:D:1221:LEU:HD22 | 3:D:1306:LEU:HB2  | 1.99                     | 0.43              |
| 1:B:29:GLU:OE1    | 1:B:200:LYS:HE2   | 2.18                     | 0.43              |
| 2:C:545:PHE:CZ    | 2:C:549:ASP:HB2   | 2.54                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:720:ARG:NH1   | 2:C:736:VAL:HG21  | 2.33                     | 0.43              |
| 2:C:1244:HIS:NE2  | 2:C:1265:PHE:O    | 2.52                     | 0.43              |
| 3:D:905:ARG:HD2   | 4:E:16:ARG:CD     | 2.48                     | 0.43              |
| 3:D:1001:ALA:HB1  | 3:D:1020:TRP:CE2  | 2.54                     | 0.43              |
| 1:B:178:SER:OG    | 1:B:180:VAL:HG22  | 2.18                     | 0.43              |
| 2:C:806:PRO:O     | 3:D:633:ALA:HA    | 2.19                     | 0.43              |
| 2:C:972:PHE:CD2   | 2:C:994:ARG:HD3   | 2.53                     | 0.43              |
| 2:C:1007:LYS:O    | 2:C:1011:LEU:HD23 | 2.18                     | 0.43              |
| 2:C:1101:LEU:HB3  | 3:D:731:ARG:CG    | 2.44                     | 0.43              |
| 2:C:1276:TRP:CG   | 3:D:801:VAL:HG11  | 2.54                     | 0.43              |
| 3:D:422:LEU:O     | 3:D:468:VAL:HA    | 2.19                     | 0.43              |
| 4:E:21:LEU:O      | 4:E:25:ARG:HG2    | 2.19                     | 0.43              |
| 1:B:210:THR:OG1   | 1:B:211:ILE:N     | 2.52                     | 0.43              |
| 2:C:179:TYR:HE2   | 2:C:462:ASN:HD21  | 1.66                     | 0.43              |
| 2:C:224:PHE:CD2   | 2:C:347:ILE:HG13  | 2.53                     | 0.43              |
| 2:C:807:TRP:HB2   | 2:C:1097:VAL:HG11 | 1.99                     | 0.43              |
| 2:C:1336:ASN:N    | 3:D:23:ALA:O      | 2.46                     | 0.43              |
| 3:D:160:LEU:HD21  | 3:D:165:TYR:HA    | 1.99                     | 0.43              |
| 3:D:179:LYS:HZ3   | 3:D:183:GLU:C     | 2.27                     | 0.43              |
| 3:D:814:CYS:SG    | 3:D:816:THR:HG22  | 2.58                     | 0.43              |
| 3:D:1348:LYS:O    | 3:D:1352:ILE:HG13 | 2.19                     | 0.43              |
| 2:C:26:TYR:HE2    | 2:C:28:LEU:HB2    | 1.82                     | 0.43              |
| 2:C:466:VAL:O     | 2:C:470:ARG:HD3   | 2.18                     | 0.43              |
| 2:C:934:PHE:HB2   | 2:C:1049:ILE:HG12 | 2.01                     | 0.43              |
| 3:D:438:GLU:OE1   | 4:E:2:ALA:HB3     | 2.17                     | 0.43              |
| 3:D:826:ILE:HG13  | 3:D:826:ILE:O     | 2.19                     | 0.43              |
| 4:E:46:THR:HA     | 4:E:49:ILE:HD12   | 2.01                     | 0.43              |
| 2:C:80:PHE:CD2    | 2:C:84:GLU:HG3    | 2.50                     | 0.43              |
| 2:C:232:ILE:O     | 2:C:232:ILE:HG13  | 2.19                     | 0.43              |
| 2:C:719:LYS:HE2   | 2:C:751:TYR:CE1   | 2.54                     | 0.43              |
| 2:C:1101:LEU:HD22 | 3:D:504:GLN:HB2   | 2.01                     | 0.43              |
| 2:C:1268:GLN:OE1  | 3:D:352:ARG:HD2   | 2.19                     | 0.43              |
| 3:D:770:LEU:O     | 3:D:774:ILE:HG13  | 2.19                     | 0.43              |
| 3:D:1028:ILE:HD13 | 3:D:1118:GLY:HA2  | 2.00                     | 0.43              |
| 3:D:1219:ASP:O    | 3:D:1223:LEU:HG   | 2.19                     | 0.43              |
| 3:D:139:LEU:CD2   | 3:D:300:GLN:HG2   | 2.49                     | 0.42              |
| 3:D:328:ALA:O     | 3:D:332:LYS:HG2   | 2.18                     | 0.42              |
| 3:D:647:PRO:HB3   | 3:D:697:MET:HA    | 2.01                     | 0.42              |
| 3:D:905:ARG:CZ    | 3:D:907:HIS:HB2   | 2.49                     | 0.42              |
| 3:D:1081:VAL:HA   | 3:D:1087:ASP:HA   | 2.01                     | 0.42              |
| 1:B:120:ASP:OD1   | 1:B:121:VAL:HG13  | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:57:PHE:CD2    | 2:C:70:TYR:HB2    | 2.54                     | 0.42              |
| 2:C:339:ASN:N     | 2:C:343:HIS:O     | 2.53                     | 0.42              |
| 2:C:369:MET:HE3   | 2:C:370:MET:HE3   | 2.00                     | 0.42              |
| 2:C:472:GLU:HA    | 2:C:475:VAL:HG12  | 2.01                     | 0.42              |
| 3:D:697:MET:HB3   | 3:D:697:MET:HE3   | 1.74                     | 0.42              |
| 2:C:138:ILE:HG13  | 2:C:143:ARG:HD2   | 2.01                     | 0.42              |
| 2:C:178:PRO:HA    | 2:C:397:LEU:HD23  | 2.01                     | 0.42              |
| 2:C:230:PHE:HB2   | 2:C:333:ILE:HB    | 2.01                     | 0.42              |
| 2:C:677:ASN:ND2   | 3:D:935:PHE:HE1   | 2.17                     | 0.42              |
| 2:C:805:MET:HE1   | 2:C:1221:PHE:CZ   | 2.54                     | 0.42              |
| 2:C:813:GLU:HB2   | 3:D:461:PHE:HD2   | 1.83                     | 0.42              |
| 3:D:611:ILE:HG22  | 3:D:612:LEU:HD12  | 2.01                     | 0.42              |
| 3:D:1148:ARG:HH11 | 5:N:20:DG:H4'     | 1.84                     | 0.42              |
| 3:D:1216:ALA:O    | 3:D:1220:ILE:HD12 | 2.19                     | 0.42              |
| 2:C:515:MET:HE2   | 2:C:515:MET:HB3   | 1.80                     | 0.42              |
| 2:C:1004:ASP:O    | 2:C:1005:GLU:HG3  | 2.19                     | 0.42              |
| 2:C:1245:ALA:HB2  | 3:D:372:MET:CG    | 2.49                     | 0.42              |
| 3:D:316:ILE:HG22  | 3:D:317:THR:N     | 2.34                     | 0.42              |
| 3:D:492:SER:OG    | 3:D:495:ASN:O     | 2.35                     | 0.42              |
| 3:D:502:PRO:HG2   | 3:D:601:ILE:HG21  | 2.01                     | 0.42              |
| 3:D:954:ASN:ND2   | 3:D:992:LYS:HG2   | 2.34                     | 0.42              |
| 3:D:1175:LEU:HB2  | 3:D:1190:ILE:CD1  | 2.49                     | 0.42              |
| 7:T:17:DC:H2'     | 7:T:18:DC:H6      | 1.84                     | 0.42              |
| 1:B:137:ASN:OD1   | 1:B:138:ALA:N     | 2.41                     | 0.42              |
| 2:C:665:ALA:HA    | 2:C:668:ILE:HD12  | 2.00                     | 0.42              |
| 2:C:813:GLU:C     | 2:C:815:SER:N     | 2.77                     | 0.42              |
| 2:C:1058:ARG:HG2  | 2:C:1058:ARG:HH11 | 1.83                     | 0.42              |
| 2:C:1075:VAL:HG23 | 3:D:463:GLY:H     | 1.85                     | 0.42              |
| 3:D:66:LYS:HB3    | 3:D:69:GLU:OE2    | 2.20                     | 0.42              |
| 3:D:126:LEU:CD1   | 3:D:223:LEU:HD22  | 2.50                     | 0.42              |
| 3:D:531:LYS:O     | 3:D:534:GLU:HG2   | 2.19                     | 0.42              |
| 3:D:1000:GLY:HA2  | 3:D:1028:ILE:HG13 | 2.01                     | 0.42              |
| 1:A:51:MET:HE1    | 1:A:219:ARG:HB3   | 2.02                     | 0.42              |
| 2:C:961:SER:HA    | 2:C:964:LEU:HD12  | 2.01                     | 0.42              |
| 3:D:143:SER:HG    | 3:D:160:LEU:C     | 2.19                     | 0.42              |
| 3:D:706:VAL:O     | 3:D:706:VAL:HG23  | 2.20                     | 0.42              |
| 3:D:1082:ASP:HB3  | 3:D:1084:GLN:OE1  | 2.20                     | 0.42              |
| 3:D:1327:GLU:O    | 3:D:1327:GLU:HG2  | 2.18                     | 0.42              |
| 1:A:102:LEU:HB3   | 1:A:142:MET:HG2   | 2.01                     | 0.42              |
| 1:B:41:ASN:HD21   | 2:C:1217:THR:HG23 | 1.84                     | 0.42              |
| 1:B:179:PRO:HG2   | 1:B:211:ILE:HD11  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:817:LEU:HD21  | 2:C:1080:ASN:ND2  | 2.34                     | 0.42              |
| 2:C:1307:ASN:OD1  | 2:C:1312:ASN:HB3  | 2.20                     | 0.42              |
| 3:D:649:LYS:O     | 3:D:653:ILE:HG13  | 2.19                     | 0.42              |
| 3:D:1155:ILE:HD12 | 3:D:1211:SER:HB3  | 2.02                     | 0.42              |
| 3:D:1261:LEU:HD13 | 3:D:1304:ARG:HH11 | 1.85                     | 0.42              |
| 2:C:241:LEU:HD12  | 2:C:242:VAL:N     | 2.35                     | 0.42              |
| 2:C:405:PHE:CE2   | 2:C:424:ASP:HB3   | 2.55                     | 0.42              |
| 2:C:452:ARG:HH22  | 2:C:458:GLU:CD    | 2.28                     | 0.42              |
| 2:C:693:LEU:HG    | 2:C:829:THR:HG23  | 2.02                     | 0.42              |
| 3:D:504:GLN:OE1   | 3:D:731:ARG:HD3   | 2.19                     | 0.42              |
| 2:C:452:ARG:HH12  | 2:C:458:GLU:CD    | 2.27                     | 0.42              |
| 2:C:557:ARG:HB3   | 2:C:587:LEU:HD13  | 2.02                     | 0.42              |
| 2:C:561:ILE:HG21  | 3:D:772:TYR:HE2   | 1.84                     | 0.42              |
| 2:C:632:ASP:O     | 2:C:647:ARG:HG2   | 2.19                     | 0.42              |
| 2:C:934:PHE:HB2   | 2:C:1049:ILE:CG1  | 2.50                     | 0.42              |
| 3:D:60:ARG:HE     | 3:D:89:GLY:H      | 1.68                     | 0.42              |
| 3:D:709:ARG:CG    | 3:D:710:ASP:H     | 2.33                     | 0.42              |
| 3:D:786:THR:HG21  | 3:D:935:PHE:HB2   | 2.02                     | 0.42              |
| 1:A:82:LEU:O      | 1:A:86:LYS:HG3    | 2.20                     | 0.42              |
| 1:A:102:LEU:HD21  | 1:A:110:VAL:HG11  | 2.01                     | 0.42              |
| 2:C:624:ASP:C     | 2:C:625:GLU:HG3   | 2.45                     | 0.42              |
| 2:C:814:ASP:OD1   | 2:C:1106:ARG:NH2  | 2.52                     | 0.42              |
| 2:C:1066:MET:HB3  | 2:C:1066:MET:HE2  | 1.74                     | 0.42              |
| 2:C:1112:ILE:HD13 | 2:C:1112:ILE:HA   | 1.86                     | 0.42              |
| 2:C:1127:LYS:HE2  | 2:C:1127:LYS:HB2  | 1.76                     | 0.42              |
| 3:D:706:VAL:HG12  | 3:D:715:LYS:HG3   | 2.02                     | 0.42              |
| 3:D:868:TRP:O     | 3:D:872:LEU:HG    | 2.20                     | 0.42              |
| 3:D:1179:PRO:HG2  | 3:D:1182:GLY:C    | 2.45                     | 0.42              |
| 2:C:662:SER:OG    | 2:C:663:VAL:N     | 2.53                     | 0.41              |
| 2:C:802:VAL:HG21  | 2:C:1230:MET:HE3  | 2.02                     | 0.41              |
| 2:C:821:ARG:HG2   | 2:C:821:ARG:HH11  | 1.85                     | 0.41              |
| 2:C:890:LYS:N     | 2:C:911:SER:O     | 2.53                     | 0.41              |
| 2:C:1023:HIS:HA   | 2:C:1026:GLU:HG3  | 2.02                     | 0.41              |
| 3:D:825:VAL:HG13  | 3:D:825:VAL:O     | 2.20                     | 0.41              |
| 3:D:1080:ILE:HD13 | 3:D:1099:TYR:CZ   | 2.55                     | 0.41              |
| 3:D:1278:GLU:OE2  | 3:D:1283:SER:HB2  | 2.19                     | 0.41              |
| 4:E:7:GLN:O       | 4:E:11:GLU:HG3    | 2.19                     | 0.41              |
| 1:A:41:ASN:O      | 1:A:45:ARG:HG2    | 2.20                     | 0.41              |
| 2:C:277:LEU:HD12  | 2:C:278:GLU:N     | 2.34                     | 0.41              |
| 2:C:1186:VAL:HG23 | 2:C:1187:PHE:H    | 1.84                     | 0.41              |
| 2:C:1282:GLY:CA   | 4:E:17:PHE:HE1    | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1339:LEU:HD23 | 3:D:20:ILE:HG12   | 2.02                     | 0.41              |
| 3:D:316:ILE:HG22  | 3:D:317:THR:H     | 1.86                     | 0.41              |
| 3:D:416:ILE:HG21  | 3:D:441:LEU:CD2   | 2.50                     | 0.41              |
| 3:D:536:LEU:HD23  | 3:D:536:LEU:HA    | 1.88                     | 0.41              |
| 3:D:646:ILE:CD1   | 3:D:762:ASN:HD21  | 2.33                     | 0.41              |
| 3:D:703:THR:HG23  | 3:D:716:GLN:C     | 2.45                     | 0.41              |
| 3:D:863:LEU:HD13  | 3:D:908:ILE:HD13  | 2.01                     | 0.41              |
| 3:D:865:HIS:CE1   | 3:D:867:GLN:HB3   | 2.55                     | 0.41              |
| 1:A:9:LEU:HD21    | 1:A:198:LEU:HD21  | 2.03                     | 0.41              |
| 1:A:118:ASP:OD1   | 1:A:119:GLY:N     | 2.54                     | 0.41              |
| 1:B:167:PRO:C     | 1:B:170:ARG:HH21  | 2.28                     | 0.41              |
| 1:B:197:ASP:C     | 1:B:198:LEU:HD12  | 2.45                     | 0.41              |
| 2:C:84:GLU:HB2    | 2:C:88:ARG:HH12   | 1.85                     | 0.41              |
| 2:C:189:ASP:OD2   | 2:C:193:ASN:HB2   | 2.21                     | 0.41              |
| 2:C:233:ARG:C     | 2:C:235:ASN:H     | 2.29                     | 0.41              |
| 2:C:540:ARG:HA    | 2:C:571:LEU:CD1   | 2.50                     | 0.41              |
| 2:C:841:ARG:HA    | 2:C:1046:VAL:HA   | 2.01                     | 0.41              |
| 2:C:1102:GLY:O    | 2:C:1106:ARG:HB2  | 2.19                     | 0.41              |
| 2:C:1243:MET:HG2  | 3:D:372:MET:HE2   | 2.03                     | 0.41              |
| 3:D:698:MET:O     | 3:D:702:GLN:CB    | 2.68                     | 0.41              |
| 3:D:905:ARG:NH2   | 3:D:907:HIS:HB2   | 2.35                     | 0.41              |
| 1:B:9:LEU:HD13    | 1:B:198:LEU:HD21  | 2.02                     | 0.41              |
| 2:C:77:GLU:O      | 2:C:77:GLU:HG2    | 2.20                     | 0.41              |
| 2:C:242:VAL:HB    | 2:C:245:ARG:CD    | 2.51                     | 0.41              |
| 3:D:127:LEU:HG    | 3:D:192:MET:HE1   | 2.03                     | 0.41              |
| 3:D:1274:PHE:O    | 3:D:1275:LEU:HD12 | 2.20                     | 0.41              |
| 2:C:228:VAL:HB    | 2:C:335:THR:HG22  | 2.03                     | 0.41              |
| 2:C:854:ILE:O     | 2:C:857:VAL:HG22  | 2.20                     | 0.41              |
| 3:D:113:HIS:HB3   | 3:D:116:PHE:HD2   | 1.85                     | 0.41              |
| 3:D:490:ILE:O     | 3:D:499:ILE:HG22  | 2.20                     | 0.41              |
| 3:D:510:LEU:HD11  | 3:D:624:ILE:HG23  | 2.03                     | 0.41              |
| 1:A:223:ILE:HA    | 1:A:226:GLU:HG2   | 2.01                     | 0.41              |
| 1:B:10:LYS:HA     | 1:B:10:LYS:HD2    | 1.52                     | 0.41              |
| 1:B:107:ILE:HD12  | 1:B:134:THR:C     | 2.46                     | 0.41              |
| 2:C:30:ILE:CD1    | 2:C:575:LEU:HD13  | 2.50                     | 0.41              |
| 2:C:315:MET:HE3   | 2:C:315:MET:HB2   | 1.98                     | 0.41              |
| 2:C:562:GLU:OE2   | 2:C:687:ARG:HD3   | 2.20                     | 0.41              |
| 2:C:948:ILE:O     | 2:C:952:GLN:HG3   | 2.20                     | 0.41              |
| 3:D:348:ASP:O     | 3:D:349:TYR:C     | 2.63                     | 0.41              |
| 3:D:905:ARG:HD2   | 4:E:16:ARG:HD3    | 2.03                     | 0.41              |
| 3:D:973:LEU:HB3   | 3:D:1003:LEU:HD22 | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1327:GLU:H    | 3:D:1327:GLU:CD   | 2.29                     | 0.41              |
| 1:A:76:GLU:OE2    | 1:A:132:HIS:HD2   | 2.04                     | 0.41              |
| 1:B:46:ILE:HD13   | 1:B:224:LEU:HB2   | 2.03                     | 0.41              |
| 1:B:180:VAL:CG1   | 1:B:205:MET:HE3   | 2.51                     | 0.41              |
| 2:C:92:TYR:CE2    | 2:C:129:LEU:HB2   | 2.56                     | 0.41              |
| 2:C:636:CYS:HB2   | 2:C:645:PHE:CD2   | 2.55                     | 0.41              |
| 3:D:45:ASN:C      | 3:D:47:ARG:N      | 2.77                     | 0.41              |
| 3:D:167:ASP:OD1   | 3:D:168:ALA:N     | 2.54                     | 0.41              |
| 3:D:981:GLU:OE2   | 3:D:994:SER:OG    | 2.21                     | 0.41              |
| 3:D:1176:VAL:HG12 | 3:D:1187:GLU:HG2  | 2.03                     | 0.41              |
| 3:D:1263:LYS:HZ2  | 3:D:1315:ALA:HB1  | 1.82                     | 0.41              |
| 4:E:45:LYS:O      | 4:E:49:ILE:HG13   | 2.20                     | 0.41              |
| 7:T:17:DC:H2'     | 7:T:18:DC:C6      | 2.54                     | 0.41              |
| 1:A:83:LEU:HD11   | 2:C:693:LEU:HD13  | 2.03                     | 0.41              |
| 2:C:148:GLN:HA    | 2:C:531:SER:O     | 2.20                     | 0.41              |
| 2:C:463:GLN:HG2   | 2:C:505:PHE:CB    | 2.49                     | 0.41              |
| 2:C:465:ARG:HG3   | 2:C:465:ARG:NH1   | 2.36                     | 0.41              |
| 2:C:611:GLU:HG3   | 2:C:616:ILE:CD1   | 2.51                     | 0.41              |
| 2:C:660:VAL:HG21  | 3:D:769:VAL:HG11  | 2.03                     | 0.41              |
| 2:C:848:GLU:HG3   | 2:C:886:LYS:CE    | 2.50                     | 0.41              |
| 2:C:994:ARG:HA    | 2:C:997:TRP:CE2   | 2.56                     | 0.41              |
| 3:D:490:ILE:HG22  | 3:D:500:ILE:HD13  | 2.01                     | 0.41              |
| 3:D:650:LYS:O     | 3:D:654:ILE:HG12  | 2.20                     | 0.41              |
| 3:D:800:LEU:HB3   | 3:D:920:ALA:HB1   | 2.02                     | 0.41              |
| 3:D:1219:ASP:HA   | 3:D:1222:ARG:NH1  | 2.36                     | 0.41              |
| 1:A:86:LYS:HG2    | 1:A:173:VAL:CG1   | 2.50                     | 0.41              |
| 1:B:207:THR:HG22  | 1:B:208:ASN:H     | 1.85                     | 0.41              |
| 2:C:270:THR:O     | 2:C:274:ILE:HG12  | 2.21                     | 0.41              |
| 2:C:371:ARG:HB3   | 2:C:374:GLU:OE2   | 2.20                     | 0.41              |
| 2:C:448:LEU:HD23  | 2:C:448:LEU:HA    | 1.85                     | 0.41              |
| 2:C:668:ILE:HG12  | 2:C:1069:ARG:O    | 2.20                     | 0.41              |
| 2:C:681:MET:C     | 2:C:685:MET:HE2   | 2.46                     | 0.41              |
| 2:C:813:GLU:O     | 2:C:815:SER:N     | 2.54                     | 0.41              |
| 2:C:830:THR:OG1   | 2:C:832:HIS:NE2   | 2.53                     | 0.41              |
| 2:C:890:LYS:HG2   | 2:C:911:SER:C     | 2.46                     | 0.41              |
| 2:C:1066:MET:SD   | 2:C:1076:ILE:HD11 | 2.60                     | 0.41              |
| 2:C:1222:GLU:O    | 2:C:1223:ARG:HG2  | 2.21                     | 0.41              |
| 2:C:1292:THR:HG22 | 2:C:1320:PRO:HG3  | 2.03                     | 0.41              |
| 2:C:1329:GLU:C    | 2:C:1329:GLU:CD   | 2.89                     | 0.41              |
| 3:D:66:LYS:HB2    | 3:D:66:LYS:HE3    | 1.76                     | 0.41              |
| 3:D:77:ARG:NH1    | 3:D:78:LEU:HB3    | 2.35                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:210:SER:HB3   | 7:T:2:DG:H3'      | 2.03                     | 0.41              |
| 3:D:278:ARG:NE    | 3:D:295:GLU:OE2   | 2.54                     | 0.41              |
| 3:D:515:ARG:O     | 3:D:545:HIS:HB2   | 2.21                     | 0.41              |
| 3:D:860:ARG:O     | 3:D:861:ASN:C     | 2.64                     | 0.41              |
| 3:D:875:ASN:CG    | 3:D:876:SER:N     | 2.79                     | 0.41              |
| 1:A:61:ILE:HG12   | 1:A:142:MET:HB3   | 2.03                     | 0.41              |
| 1:A:166:ARG:HD3   | 1:A:166:ARG:H     | 1.86                     | 0.41              |
| 2:C:207:THR:HG21  | 2:C:351:LEU:CD2   | 2.50                     | 0.41              |
| 2:C:570:GLY:HA2   | 3:D:780:ARG:NH1   | 2.35                     | 0.41              |
| 2:C:1186:VAL:HG23 | 2:C:1187:PHE:N    | 2.36                     | 0.41              |
| 2:C:1247:SER:HB3  | 3:D:375:GLU:O     | 2.21                     | 0.41              |
| 2:C:1285:TYR:HB2  | 3:D:479:GLU:OE2   | 2.20                     | 0.41              |
| 3:D:132:LEU:HD12  | 3:D:132:LEU:HA    | 1.83                     | 0.41              |
| 3:D:861:ASN:C     | 3:D:861:ASN:HD22  | 2.19                     | 0.41              |
| 2:C:9:LYS:O       | 2:C:1175:ASN:ND2  | 2.47                     | 0.40              |
| 2:C:69:GLN:OE1    | 2:C:101:ARG:HD2   | 2.21                     | 0.40              |
| 2:C:538:LEU:HD11  | 2:C:547:VAL:HG11  | 2.03                     | 0.40              |
| 2:C:587:LEU:HD23  | 2:C:587:LEU:HA    | 1.80                     | 0.40              |
| 2:C:802:VAL:HA    | 2:C:1096:ILE:O    | 2.21                     | 0.40              |
| 2:C:1088:ASP:OD2  | 2:C:1210:ILE:HG21 | 2.21                     | 0.40              |
| 2:C:1113:LEU:HA   | 2:C:1113:LEU:HD23 | 1.89                     | 0.40              |
| 3:D:203:GLU:HA    | 3:D:203:GLU:OE1   | 2.21                     | 0.40              |
| 3:D:429:LEU:HD23  | 3:D:429:LEU:HA    | 1.66                     | 0.40              |
| 3:D:572:THR:HG21  | 3:D:589:TYR:HE2   | 1.84                     | 0.40              |
| 3:D:821:MET:CE    | 3:D:881:LYS:HB2   | 2.51                     | 0.40              |
| 3:D:1173:ARG:HD2  | 3:D:1173:ARG:C    | 2.46                     | 0.40              |
| 1:A:9:LEU:HG      | 1:A:10:LYS:N      | 2.36                     | 0.40              |
| 2:C:883:LEU:HA    | 2:C:883:LEU:HD23  | 1.81                     | 0.40              |
| 2:C:1010:GLN:O    | 2:C:1014:LEU:HG   | 2.21                     | 0.40              |
| 2:C:1072:ASN:OD1  | 2:C:1072:ASN:N    | 2.51                     | 0.40              |
| 2:C:1253:LEU:HD13 | 6:R:11:C:C1'      | 2.50                     | 0.40              |
| 3:D:146:VAL:HG22  | 3:D:158:GLN:HB3   | 2.03                     | 0.40              |
| 3:D:582:ILE:HG13  | 3:D:583:VAL:N     | 2.36                     | 0.40              |
| 3:D:801:VAL:HG13  | 3:D:917:VAL:HG13  | 2.03                     | 0.40              |
| 3:D:966:VAL:HG13  | 3:D:1030:GLU:OE2  | 2.21                     | 0.40              |
| 3:D:1137:GLY:H    | 3:D:1240:VAL:HG13 | 1.86                     | 0.40              |
| 4:E:47:THR:O      | 4:E:51:LEU:HD13   | 2.21                     | 0.40              |
| 7:T:1:DG:H2''     | 7:T:2:DG:C8       | 2.57                     | 0.40              |
| 1:A:61:ILE:HB     | 1:A:64:VAL:HG22   | 2.04                     | 0.40              |
| 2:C:28:LEU:HD13   | 2:C:527:LYS:HD3   | 2.02                     | 0.40              |
| 2:C:682:GLY:HA2   | 2:C:685:MET:HE2   | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:1018:TYR:HE1 | 2:C:1022:LYS:NZ  | 2.19                     | 0.40              |
| 2:C:1240:ASP:OD1 | 2:C:1241:ASP:N   | 2.53                     | 0.40              |
| 2:C:1315:MET:HG2 | 2:C:1316:GLU:N   | 2.36                     | 0.40              |
| 3:D:701:LEU:HD21 | 3:D:723:TYR:HB2  | 2.03                     | 0.40              |
| 1:A:175:ALA:HB1  | 1:A:177:TYR:CE1  | 2.57                     | 0.40              |
| 1:B:151:GLY:O    | 1:B:177:TYR:HB2  | 2.20                     | 0.40              |
| 2:C:93:SER:HA    | 2:C:128:PRO:HA   | 2.02                     | 0.40              |
| 2:C:520:PRO:HB2  | 2:C:794:LEU:HD11 | 2.03                     | 0.40              |
| 2:C:1292:THR:OG1 | 2:C:1293:VAL:N   | 2.54                     | 0.40              |
| 3:D:225:GLU:HA   | 3:D:228:VAL:HG22 | 2.03                     | 0.40              |
| 3:D:596:LEU:HD21 | 3:D:604:MET:HE3  | 2.03                     | 0.40              |
| 3:D:822:MET:HE3  | 3:D:838:ARG:NE   | 2.37                     | 0.40              |
| 1:A:45:ARG:HH22  | 1:B:37:HIS:HB2   | 1.87                     | 0.40              |
| 2:C:865:LEU:HD22 | 2:C:869:GLY:C    | 2.47                     | 0.40              |
| 2:C:888:THR:OG1  | 2:C:916:SER:HB3  | 2.22                     | 0.40              |
| 3:D:111:THR:CG2  | 3:D:303:VAL:HG11 | 2.37                     | 0.40              |
| 3:D:167:ASP:O    | 3:D:170:GLU:HG2  | 2.21                     | 0.40              |
| 3:D:665:GLN:OE1  | 3:D:665:GLN:HA   | 2.21                     | 0.40              |
| 3:D:710:ASP:OD1  | 3:D:711:GLY:N    | 2.49                     | 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     | 229/237 (97%)   | 213 (93%)  | 16 (7%)  | 0        | 100         | 100 |
| 1   | B     | 228/237 (96%)   | 209 (92%)  | 17 (8%)  | 2 (1%)   | 14          | 43  |
| 2   | C     | 1316/1340 (98%) | 1209 (92%) | 99 (8%)  | 8 (1%)   | 21          | 52  |
| 3   | D     | 1338/1363 (98%) | 1219 (91%) | 114 (8%) | 5 (0%)   | 30          | 59  |
| 4   | E     | 67/91 (74%)     | 61 (91%)   | 6 (9%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| All | All   | 3178/3268 (97%) | 2911 (92%) | 252 (8%) | 15 (0%)  | 26          | 55 |

All (15) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 21   | SER  |
| 2   | C     | 199  | ASP  |
| 2   | C     | 913  | VAL  |
| 2   | C     | 1041 | ASP  |
| 3   | D     | 338  | PHE  |
| 3   | D     | 1345 | ARG  |
| 2   | C     | 398  | SER  |
| 1   | B     | 193  | GLU  |
| 2   | C     | 625  | GLU  |
| 2   | C     | 1317 | PRO  |
| 2   | C     | 43   | PRO  |
| 3   | D     | 46   | TYR  |
| 3   | D     | 860  | ARG  |
| 3   | D     | 1151 | LYS  |
| 2   | C     | 1223 | ARG  |

### 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     | 199/204 (98%)   | 199 (100%) | 0        | 100         | 100 |
| 1   | B     | 198/204 (97%)   | 194 (98%)  | 4 (2%)   | 48          | 68  |
| 2   | C     | 1139/1155 (99%) | 1118 (98%) | 21 (2%)  | 51          | 70  |
| 3   | D     | 1117/1136 (98%) | 1109 (99%) | 8 (1%)   | 76          | 80  |
| 4   | E     | 59/75 (79%)     | 59 (100%)  | 0        | 100         | 100 |
| All | All   | 2712/2774 (98%) | 2679 (99%) | 33 (1%)  | 61          | 74  |

All (33) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 10   | LYS  |
| 1   | B     | 13   | LEU  |
| 1   | B     | 14   | VAL  |
| 1   | B     | 15   | ASP  |
| 2   | C     | 104  | ILE  |
| 2   | C     | 106  | GLU  |
| 2   | C     | 107  | ARG  |
| 2   | C     | 111  | GLU  |
| 2   | C     | 113  | THR  |
| 2   | C     | 114  | VAL  |
| 2   | C     | 214  | ASN  |
| 2   | C     | 935  | THR  |
| 2   | C     | 936  | ARG  |
| 2   | C     | 937  | ASP  |
| 2   | C     | 939  | VAL  |
| 2   | C     | 940  | GLU  |
| 2   | C     | 941  | LYS  |
| 2   | C     | 943  | LYS  |
| 2   | C     | 1158 | LYS  |
| 2   | C     | 1160 | ASP  |
| 2   | C     | 1161 | LEU  |
| 2   | C     | 1165 | SER  |
| 2   | C     | 1170 | MET  |
| 2   | C     | 1171 | ARG  |
| 2   | C     | 1315 | MET  |
| 3   | D     | 52   | GLU  |
| 3   | D     | 53   | ARG  |
| 3   | D     | 54   | ASP  |
| 3   | D     | 56   | LEU  |
| 3   | D     | 157  | GLN  |
| 3   | D     | 861  | ASN  |
| 3   | D     | 1289 | ASN  |
| 3   | D     | 1301 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 41  | ASN  |
| 1   | A     | 132 | HIS  |
| 1   | B     | 41  | ASN  |
| 1   | B     | 93  | GLN  |
| 1   | B     | 227 | GLN  |
| 2   | C     | 41  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 46   | GLN  |
| 2   | C     | 618  | GLN  |
| 2   | C     | 620  | ASN  |
| 2   | C     | 649  | GLN  |
| 2   | C     | 677  | ASN  |
| 2   | C     | 761  | GLN  |
| 2   | C     | 932  | GLN  |
| 2   | C     | 955  | GLN  |
| 2   | C     | 1010 | GLN  |
| 2   | C     | 1023 | HIS  |
| 2   | C     | 1080 | ASN  |
| 2   | C     | 1257 | GLN  |
| 2   | C     | 1313 | HIS  |
| 3   | D     | 80   | HIS  |
| 3   | D     | 229  | GLN  |
| 3   | D     | 276  | ASN  |
| 3   | D     | 341  | ASN  |
| 3   | D     | 458  | ASN  |
| 3   | D     | 594  | GLN  |
| 3   | D     | 1098 | GLN  |
| 3   | D     | 1108 | GLN  |
| 3   | D     | 1279 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 6   | R     | 10/11 (90%) | 2 (20%)           | 0               |

All (2) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | R     | 11  | C    |
| 6   | R     | 12  | G    |

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 10  | 2TM  | D     | 2004 | -    | 26,30,30     | 2.88 | 10 (38%)    | 39,47,47    | 1.12 | 4 (10%)     |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 10  | 2TM  | D     | 2004 | -    | -       | 6/19/38/38 | 0/2/2/2 |

All (10) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 10  | D     | 2004 | 2TM  | O2-C2   | 8.57  | 1.39        | 1.23     |
| 10  | D     | 2004 | 2TM  | PB-O3B  | 6.14  | 1.65        | 1.58     |
| 10  | D     | 2004 | 2TM  | C4-N4   | 4.83  | 1.45        | 1.33     |
| 10  | D     | 2004 | 2TM  | C2-N3   | 3.98  | 1.44        | 1.36     |
| 10  | D     | 2004 | 2TM  | O4'-C1' | 3.71  | 1.50        | 1.42     |
| 10  | D     | 2004 | 2TM  | C2'-C3' | -3.18 | 1.44        | 1.53     |
| 10  | D     | 2004 | 2TM  | O4'-C4' | 2.59  | 1.50        | 1.45     |
| 10  | D     | 2004 | 2TM  | C1'-N1  | -2.40 | 1.40        | 1.47     |
| 10  | D     | 2004 | 2TM  | PA-O2A  | -2.08 | 1.51        | 1.56     |
| 10  | D     | 2004 | 2TM  | C3'-C4' | -2.07 | 1.47        | 1.53     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 10  | D     | 2004 | 2TM  | C3'-C2'-C1' | 2.89  | 106.93      | 101.46   |
| 10  | D     | 2004 | 2TM  | PB-O3B-PG   | -2.78 | 122.49      | 132.45   |
| 10  | D     | 2004 | 2TM  | C4'-O4'-C1' | -2.19 | 104.62      | 109.47   |
| 10  | D     | 2004 | 2TM  | C2'-C3'-C4' | 2.09  | 106.64      | 102.61   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

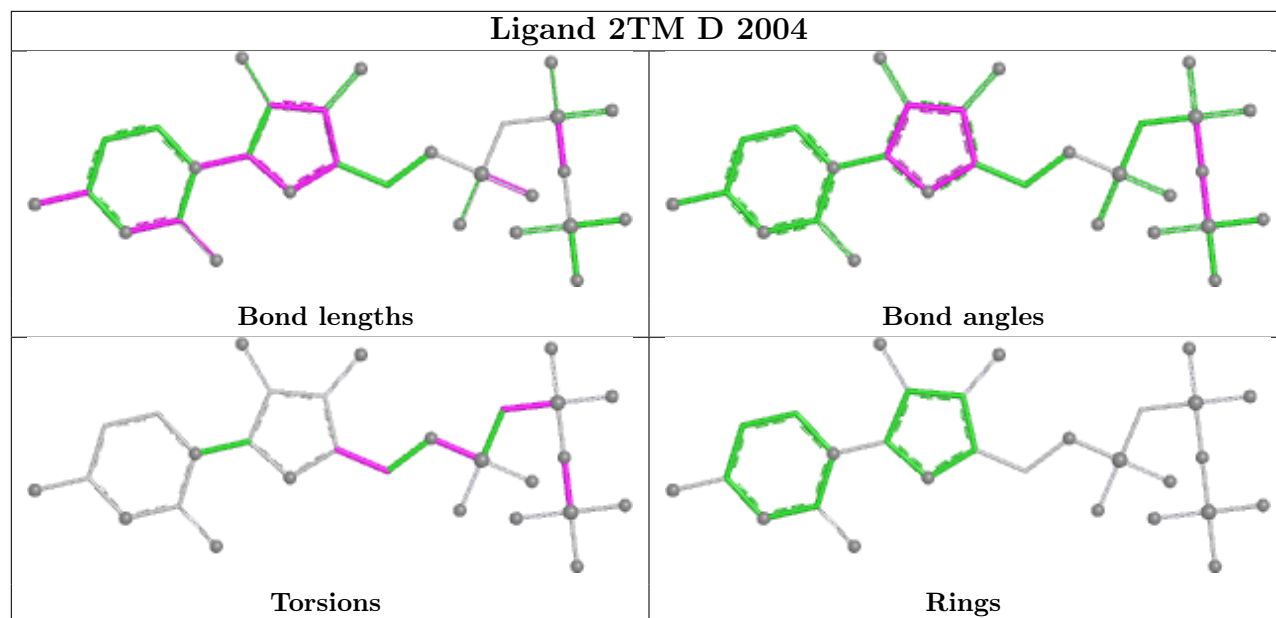
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 10  | D     | 2004 | 2TM  | C5'-O5'-PA-O1A  |
| 10  | D     | 2004 | 2TM  | PA-C1-PB-O3B    |
| 10  | D     | 2004 | 2TM  | PA-C1-PB-O1B    |
| 10  | D     | 2004 | 2TM  | PA-C1-PB-O2B    |
| 10  | D     | 2004 | 2TM  | O4'-C4'-C5'-O5' |
| 10  | D     | 2004 | 2TM  | PB-O3B-PG-O1G   |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 10  | D     | 2004 | 2TM  | 2       | 0            |

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

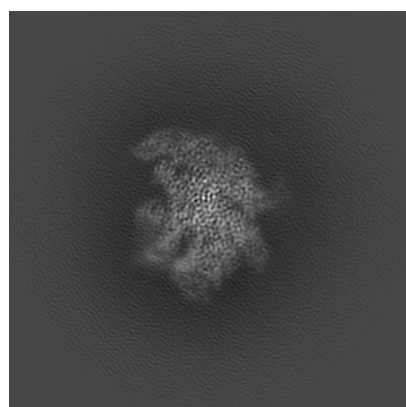
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23901. These allow visual inspection of the internal detail of the map and identification of artifacts.

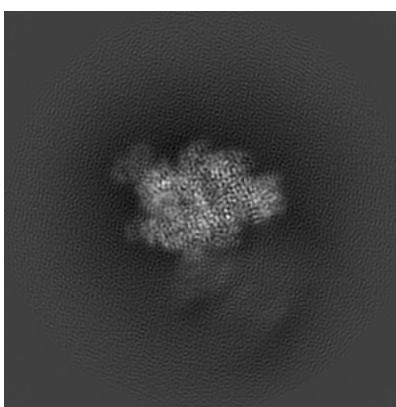
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

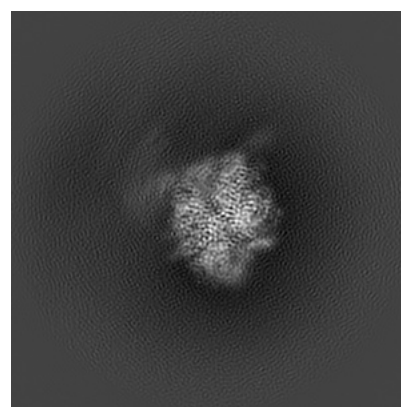
#### 6.1.1 Primary map



X



Y

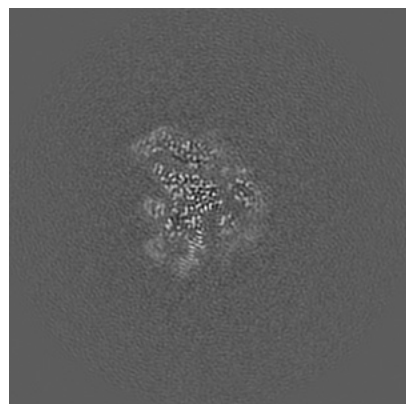


Z

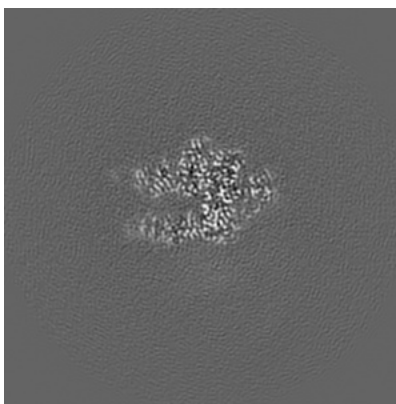
The images above show the map projected in three orthogonal directions.

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

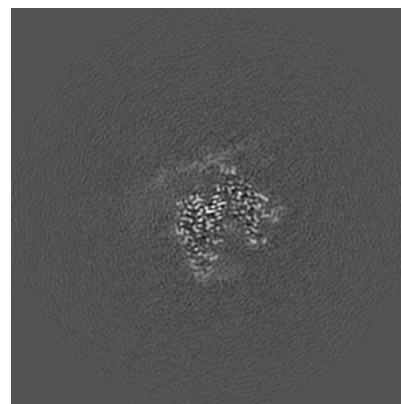
#### 6.2.1 Primary map



X Index: 130



Y Index: 130

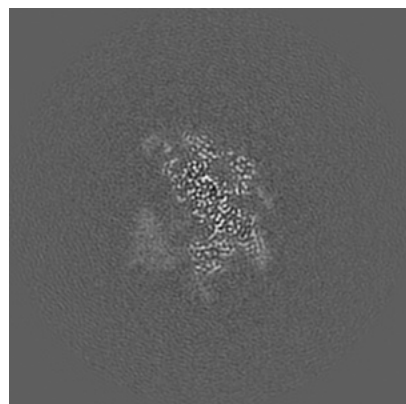


Z Index: 130

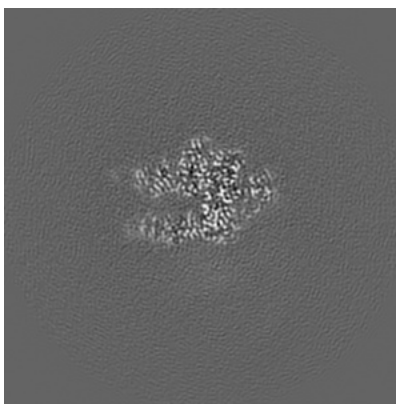
The images above show central slices of the map in three orthogonal directions.

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

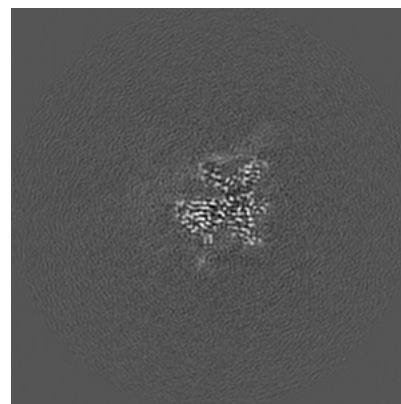
### 6.3.1 Primary map



X Index: 147



Y Index: 130

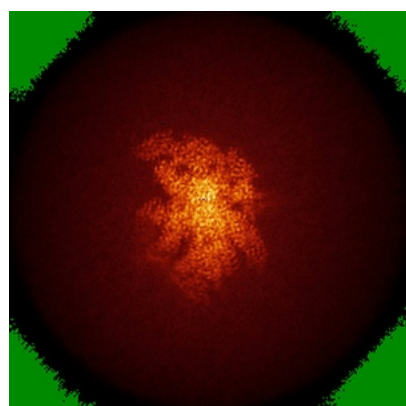


Z Index: 138

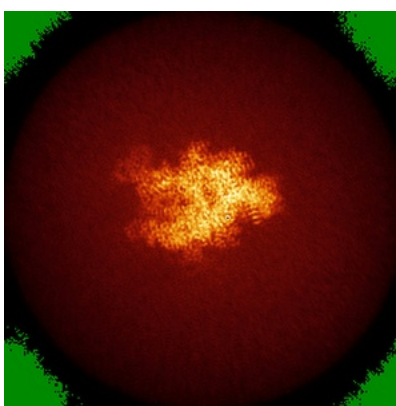
The images above show the largest variance slices of the map in three orthogonal directions.

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

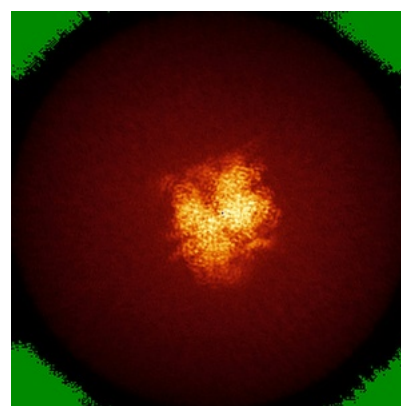
### 6.4.1 Primary map



X



Y

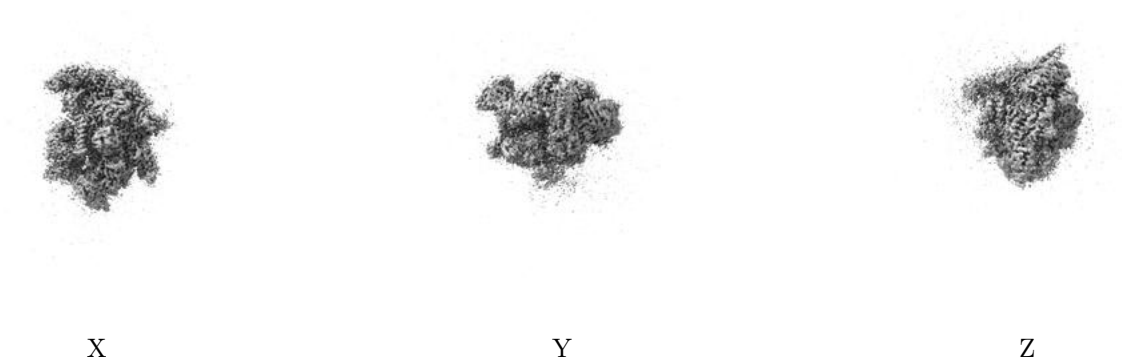


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

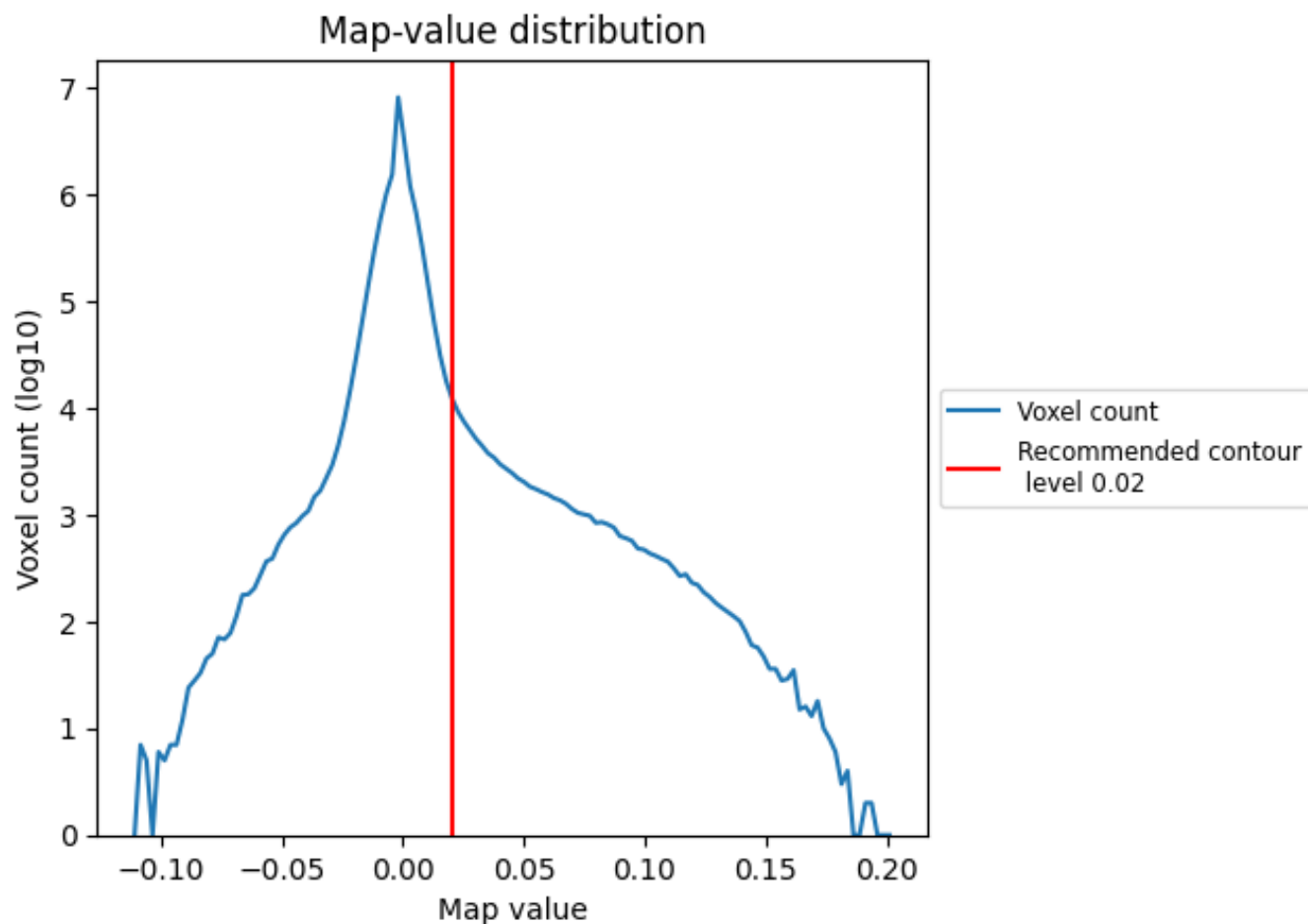
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

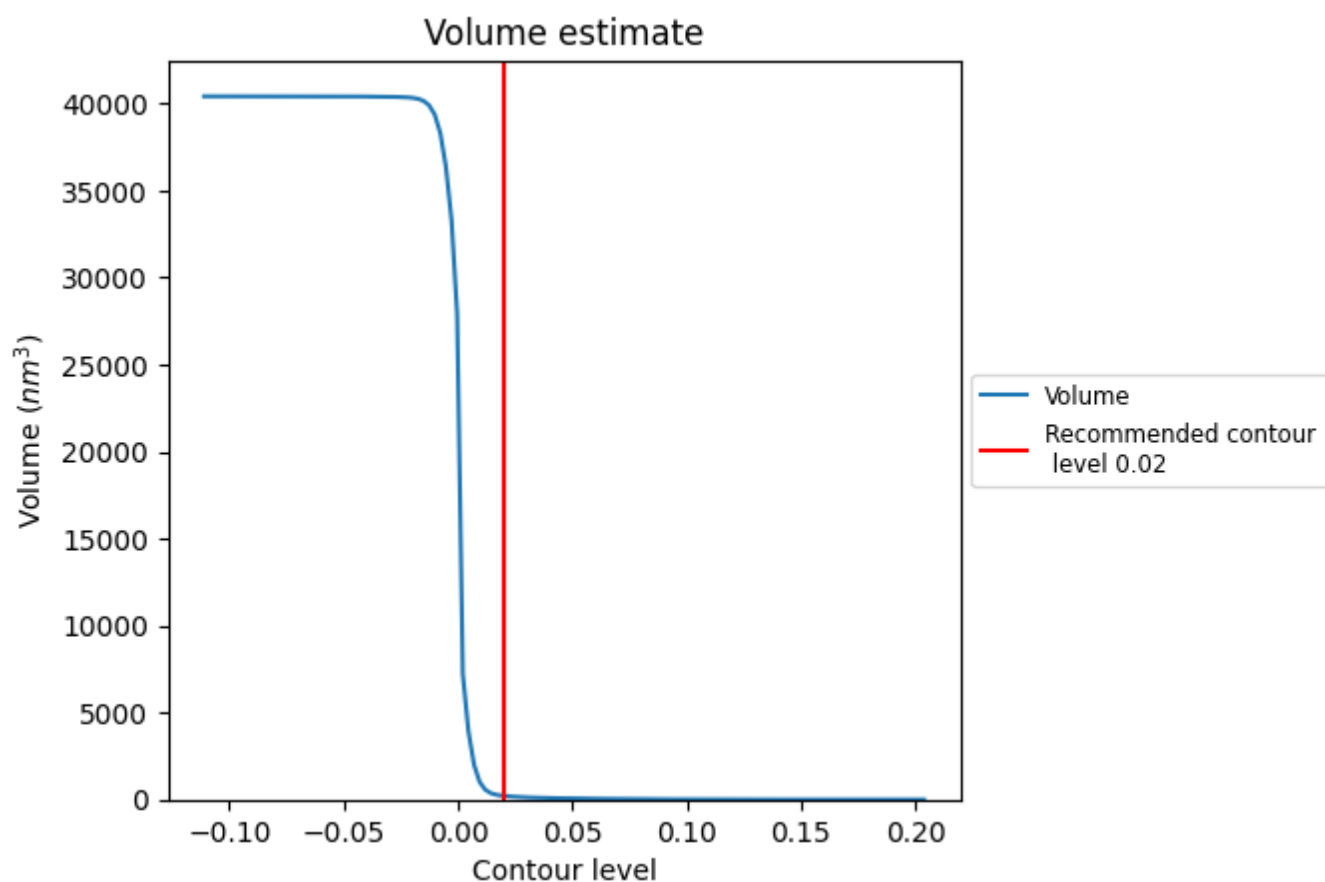
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

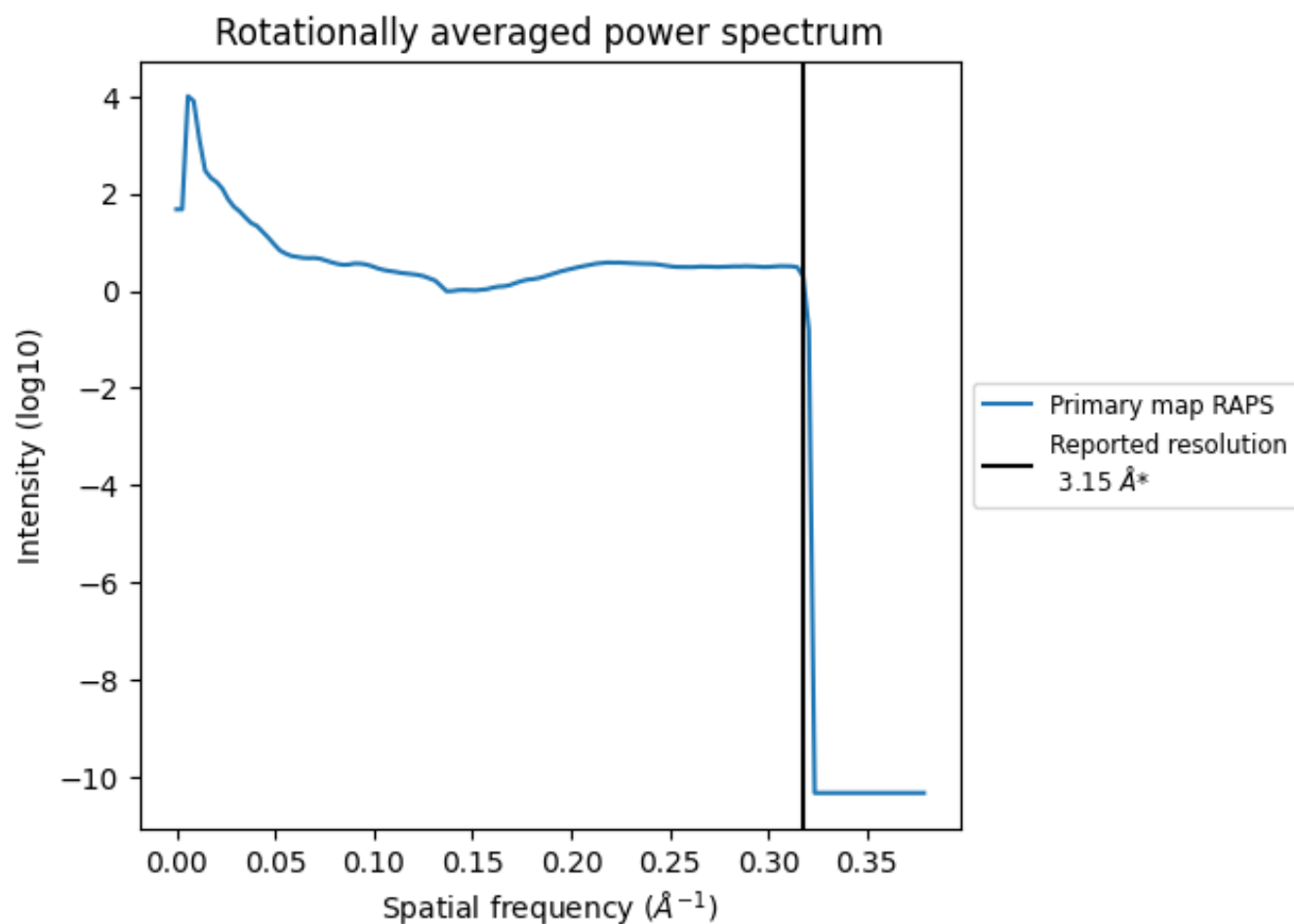
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 211  $\text{nm}^3$ ; this corresponds to an approximate mass of 191 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.317 Å<sup>-1</sup>

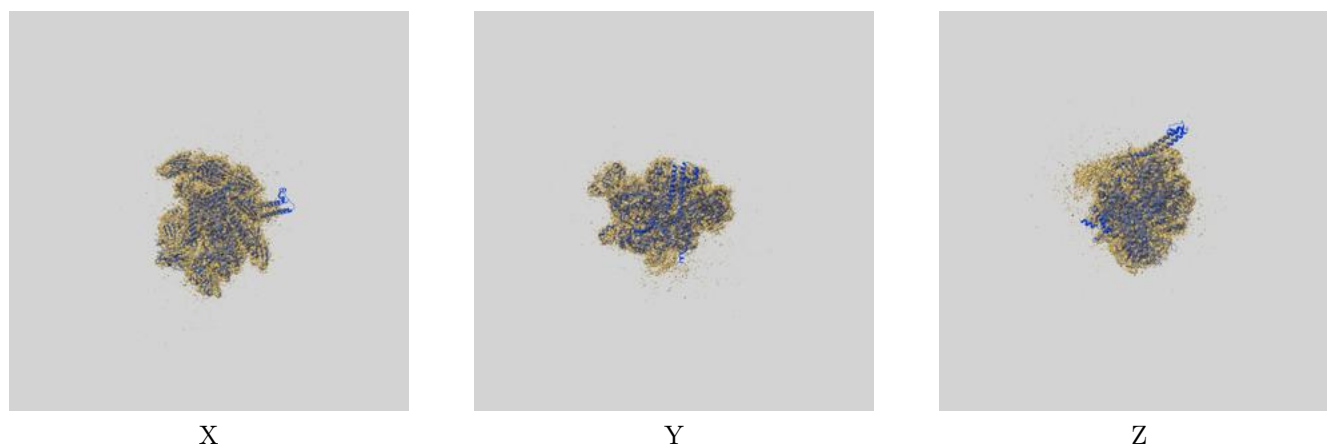
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

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

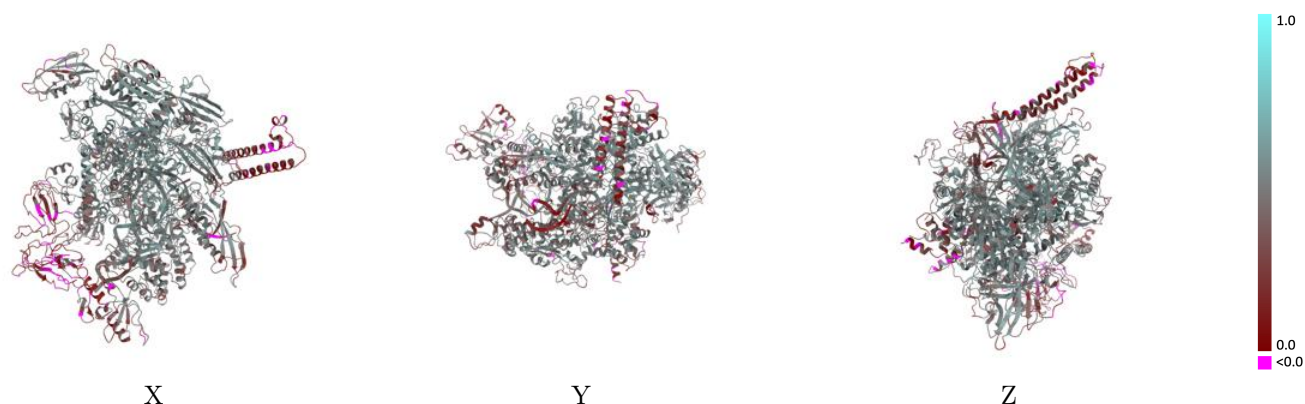
This section contains information regarding the fit between EMDB map EMD-23901 and PDB model 7MKO. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



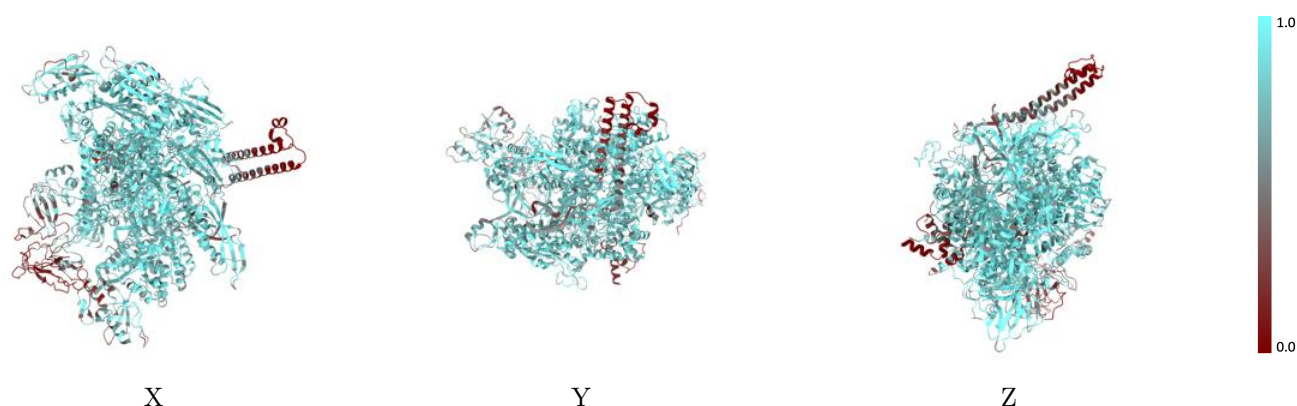
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



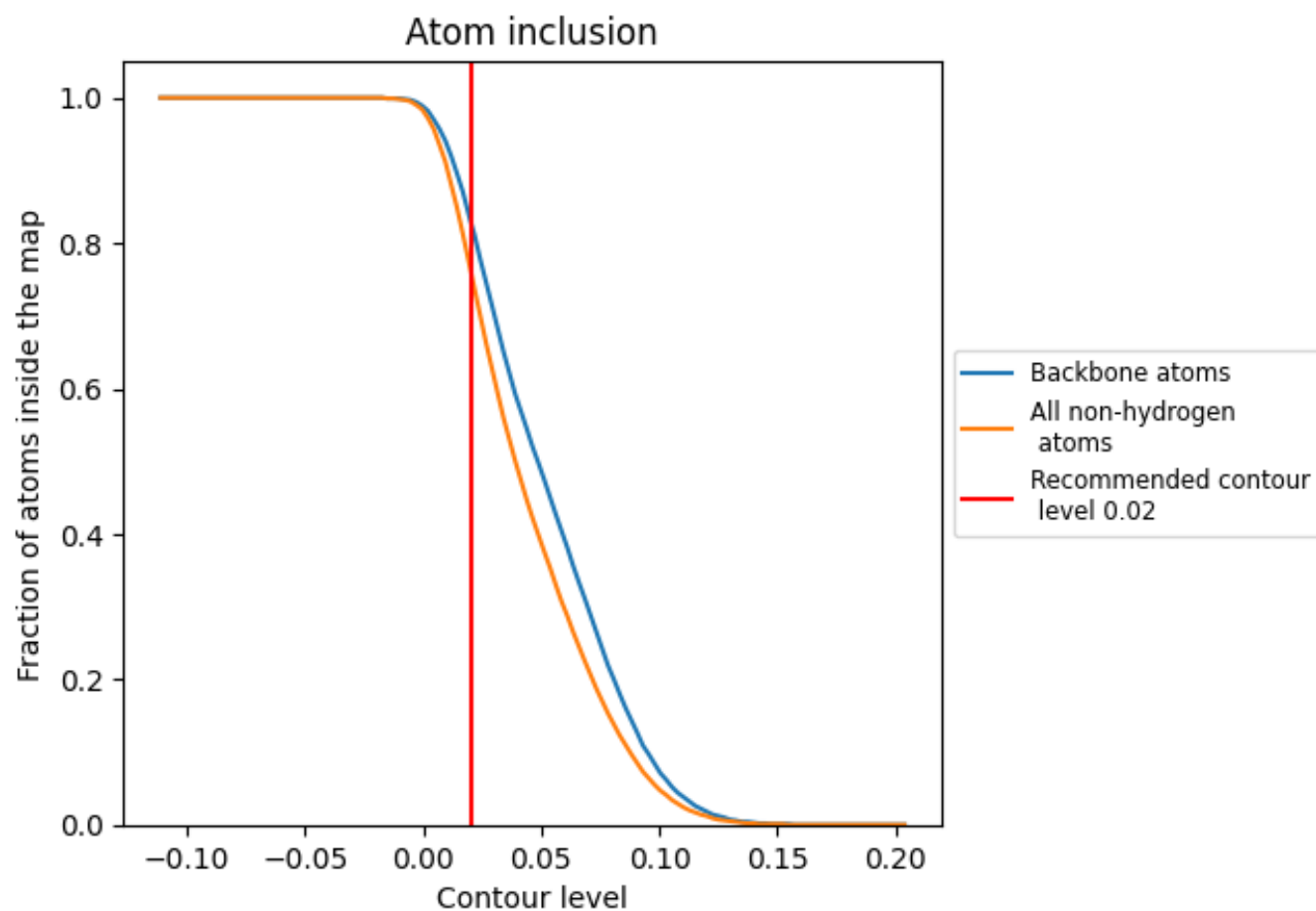
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.7640 | <div></div> 0.4330 |
| A     | <div></div> 0.8250 | <div></div> 0.4790 |
| B     | <div></div> 0.7840 | <div></div> 0.4440 |
| C     | <div></div> 0.7920 | <div></div> 0.4520 |
| D     | <div></div> 0.7490 | <div></div> 0.4170 |
| E     | <div></div> 0.1430 | <div></div> 0.2290 |
| N     | <div></div> 0.7780 | <div></div> 0.3800 |
| R     | <div></div> 0.8970 | <div></div> 0.5160 |
| T     | <div></div> 0.7750 | <div></div> 0.4030 |

1.0

0.0

<0.0