



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:34 PM UTC

PDB ID : 7QXI / pdb\_00007qxi  
EMDB ID : EMD-14200  
Title : Cryo-EM structure of RNA polymerase-sigma54 holo enzyme with promoter  
DNA closed complex  
Authors : Ye, F.Z.; Zhang, X.D.  
Deposited on : 2022-01-26  
Resolution : 3.40 Å(reported)  
Based on initial model : 5NSR

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:

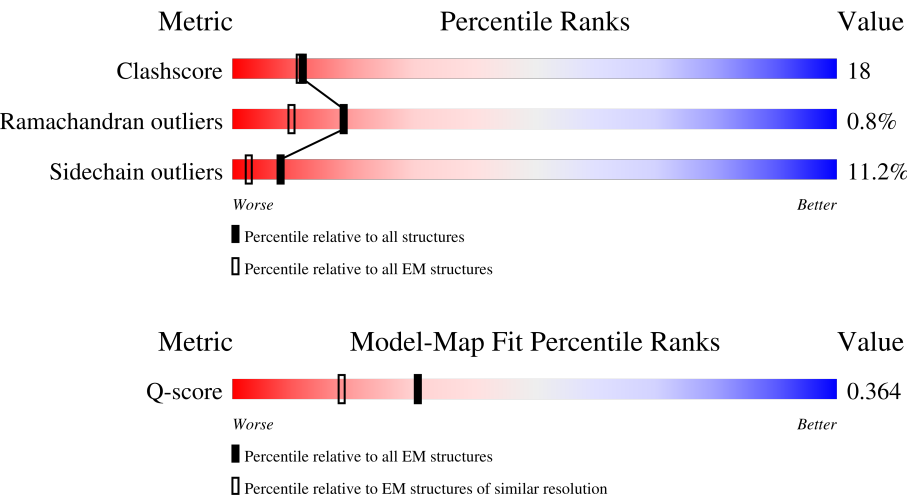
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14717 ( 2.90 - 3.90 )                                    |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 329    |                  |
| 1   | B     | 329    |                  |
| 2   | C     | 1342   |                  |
| 3   | D     | 1407   |                  |

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| Mol | Chain | Length | Quality of chain                                                                             |
|-----|-------|--------|----------------------------------------------------------------------------------------------|
| 4   | E     | 91     | <div><div></div><div>74%</div><div>7%</div><div>•</div><div>19%</div></div>                  |
| 5   | M     | 497    | <div><div>6%</div><div>32%</div><div>29%</div><div>18%</div><div>•</div><div>19%</div></div> |
| 6   | N     | 63     | <div><div>5%</div><div>35%</div><div>19%</div><div>•</div><div>43%</div></div>               |
| 7   | T     | 63     | <div><div>10%</div><div>22%</div><div>33%</div><div>•</div><div>43%</div></div>              |

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 28928 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     | 309      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2316  | 1450 | 404 | 455 | 7 |         |       |
| 1   | B     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1671  | 1042 | 293 | 331 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | C     | 1341     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10125 | 6360 | 1761 | 1964 | 40 |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 3   | D     | 1334     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9632  | 6049 | 1730 | 1814 | 39 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | E     | 74       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 546   | 335 | 109 | 101 | 1 |         |       |

- Molecule 5 is a protein called RNA polymerase sigma-54 factor.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | M     | 403      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3162  | 1974 | 551 | 626 | 11 |         |       |

There are 22 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference      |
|-------|---------|----------|--------|-----------------------|----------------|
| M     | -19     | MET      | -      | initiating methionine | UNP A0A0N9UTC1 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| M     | -18     | GLY      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -17     | SER      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -16     | SER      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -15     | HIS      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -14     | HIS      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -13     | HIS      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -12     | HIS      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -11     | HIS      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -10     | HIS      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -9      | SER      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -8      | SER      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -7      | GLY      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -6      | LEU      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -5      | VAL      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -4      | PRO      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -3      | ARG      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -2      | GLY      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | -1      | SER      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | 0       | HIS      | -      | expression tag | UNP A0A0N9UTC1 |
| M     | 49      | GLU      | GLN    | conflict       | UNP A0A0N9UTC1 |
| M     | 80      | GLU      | ASP    | conflict       | UNP A0A0N9UTC1 |

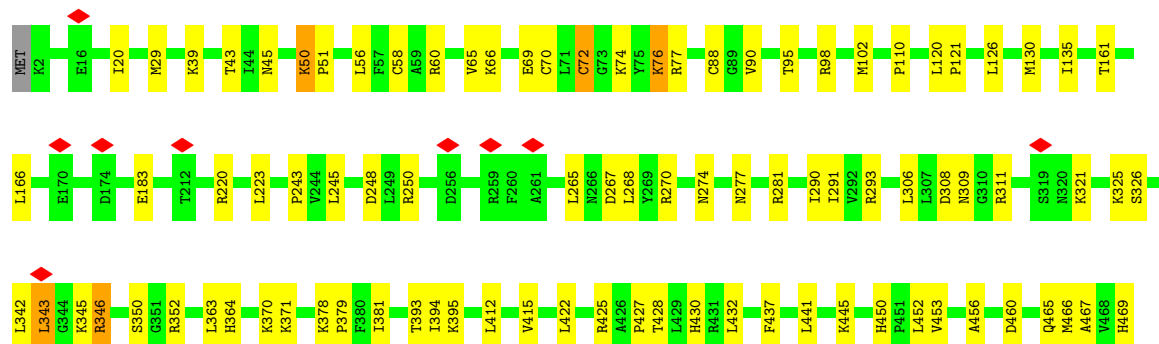
- Molecule 6 is a DNA chain called Non-Template promoter DNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 6   | N     | 36       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 738   | 349 | 137 | 216 | 36 |         |       |

- Molecule 7 is a DNA chain called Template DNA promoter.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7   | T     | 36       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 738   | 349 | 137 | 216 | 36 |         |       |









## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 29321                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 1400                                    | Depositor |
| Maximum defocus (nm)                 | 2600                                    | Depositor |
| Magnification                        | 81000                                   | Depositor |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.216                                   | Depositor |
| Minimum map value                    | -0.119                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.006                                   | Depositor |
| Recommended contour level            | 0.02                                    | Depositor |
| Map size (Å)                         | 281.6, 281.6, 281.6                     | wwPDB     |
| Map dimensions                       | 256, 256, 256                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.1, 1.1, 1.1                           | Depositor |

## 5 Model quality [i](#)

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

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     | 0.15         | 0/2345          | 0.42        | 0/3195          |
| 1   | B     | 0.14         | 0/1688          | 0.43        | 0/2293          |
| 2   | C     | 0.19         | 0/10283         | 0.51        | 4/13940 (0.0%)  |
| 3   | D     | 0.15         | 0/9766          | 0.45        | 0/13267         |
| 4   | E     | 0.14         | 0/547           | 0.52        | 1/740 (0.1%)    |
| 5   | M     | 0.98         | 15/3204 (0.5%)  | 1.22        | 22/4339 (0.5%)  |
| 6   | N     | 0.46         | 2/827 (0.2%)    | 0.92        | 4/1274 (0.3%)   |
| 7   | T     | 0.40         | 0/827           | 0.78        | 1/1274 (0.1%)   |
| All | All   | 0.37         | 17/29487 (0.1%) | 0.63        | 32/40322 (0.1%) |

All (17) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | M     | 258 | PRO  | CA-C    | -9.71 | 1.41        | 1.52     |
| 6   | N     | -10 | DG   | C4'-O4' | 7.75  | 1.60        | 1.45     |
| 5   | M     | 203 | LEU  | CA-C    | -7.47 | 1.42        | 1.52     |
| 5   | M     | 48  | GLU  | C-O     | -6.74 | 1.15        | 1.23     |
| 5   | M     | 44  | ASN  | CA-C    | -6.20 | 1.43        | 1.52     |
| 5   | M     | 368 | ALA  | CA-C    | 5.53  | 1.59        | 1.52     |
| 5   | M     | 44  | ASN  | N-CA    | 5.42  | 1.52        | 1.46     |
| 5   | M     | 258 | PRO  | C-O     | 5.42  | 1.30        | 1.23     |
| 5   | M     | 420 | ILE  | N-CA    | 5.39  | 1.52        | 1.46     |
| 5   | M     | 376 | MET  | N-CA    | 5.36  | 1.52        | 1.45     |
| 5   | M     | 46  | LEU  | N-CA    | -5.31 | 1.39        | 1.46     |
| 5   | M     | 361 | TYR  | C-O     | 5.24  | 1.29        | 1.23     |
| 5   | M     | 377 | HIS  | CA-C    | 5.16  | 1.59        | 1.52     |
| 5   | M     | 287 | VAL  | CA-C    | 5.15  | 1.59        | 1.52     |
| 5   | M     | 160 | ASP  | CA-C    | -5.09 | 1.46        | 1.52     |
| 6   | N     | -13 | DC   | C4'-O4' | -5.03 | 1.35        | 1.45     |
| 5   | M     | 380 | THR  | N-CA    | 5.01  | 1.52        | 1.46     |

All (32) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 6   | N     | -10 | DG   | O3'-P-O5'   | -14.19 | 82.72       | 104.00   |
| 5   | M     | 44  | ASN  | CB-CA-C     | -9.49  | 101.89      | 110.44   |
| 2   | C     | 896 | THR  | CA-C-N      | 8.79   | 130.82      | 119.84   |
| 2   | C     | 896 | THR  | C-N-CA      | 8.79   | 130.82      | 119.84   |
| 6   | N     | -10 | DG   | C5'-C4'-O4' | -8.61  | 96.49       | 109.40   |
| 5   | M     | 24  | ARG  | N-CA-C      | -7.37  | 103.25      | 114.16   |
| 5   | M     | 286 | THR  | N-CA-C      | 7.24   | 117.52      | 108.19   |
| 5   | M     | 16  | THR  | CB-CA-C     | -7.13  | 98.77       | 108.68   |
| 5   | M     | 258 | PRO  | CB-CA-C     | -6.92  | 101.04      | 110.60   |
| 6   | N     | -13 | DC   | C5'-C4'-O4' | 6.51   | 119.17      | 109.40   |
| 5   | M     | 47  | LEU  | CB-CA-C     | -6.35  | 100.33      | 110.81   |
| 5   | M     | 16  | THR  | N-CA-C      | 6.31   | 119.02      | 110.31   |
| 7   | T     | 10  | DC   | O4'-C4'-C3' | -6.04  | 96.34       | 105.40   |
| 5   | M     | 44  | ASN  | CA-C-O      | -5.99  | 114.86      | 119.71   |
| 5   | M     | 16  | THR  | CA-C-N      | -5.95  | 112.40      | 119.84   |
| 5   | M     | 16  | THR  | C-N-CA      | -5.95  | 112.40      | 119.84   |
| 5   | M     | 158 | ILE  | CB-CA-C     | -5.93  | 104.29      | 112.24   |
| 5   | M     | 438 | SER  | N-CA-C      | 5.79   | 117.02      | 108.86   |
| 5   | M     | 250 | VAL  | CB-CA-C     | -5.75  | 104.50      | 112.04   |
| 5   | M     | 350 | GLN  | N-CA-C      | -5.73  | 105.99      | 112.87   |
| 5   | M     | 164 | SER  | CA-C-O      | 5.56   | 126.01      | 119.28   |
| 5   | M     | 205 | GLN  | N-CA-CB     | 5.49   | 119.64      | 110.41   |
| 2   | C     | 920 | VAL  | CA-C-N      | 5.40   | 126.59      | 119.84   |
| 2   | C     | 920 | VAL  | C-N-CA      | 5.40   | 126.59      | 119.84   |
| 5   | M     | 419 | ALA  | CA-C-N      | 5.37   | 127.52      | 120.60   |
| 5   | M     | 419 | ALA  | C-N-CA      | 5.37   | 127.52      | 120.60   |
| 5   | M     | 253 | ILE  | CA-CB-CG2   | 5.33   | 119.56      | 110.50   |
| 6   | N     | -10 | DG   | C1'-O4'-C4' | -5.31  | 101.73      | 109.70   |
| 5   | M     | 417 | SER  | N-CA-CB     | 5.31   | 119.05      | 110.40   |
| 4   | E     | 6   | VAL  | N-CA-C      | -5.08  | 108.34      | 113.47   |
| 5   | M     | 46  | LEU  | CA-C-N      | -5.07  | 115.68      | 122.42   |
| 5   | M     | 46  | LEU  | C-N-CA      | -5.07  | 115.68      | 122.42   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2316  | 0        | 2297     | 55      | 0            |
| 1   | B     | 1671  | 0        | 1674     | 32      | 0            |
| 2   | C     | 10125 | 0        | 9829     | 297     | 0            |
| 3   | D     | 9632  | 0        | 9238     | 119     | 0            |
| 4   | E     | 546   | 0        | 548      | 5       | 0            |
| 5   | M     | 3162  | 0        | 3169     | 517     | 0            |
| 6   | N     | 738   | 0        | 404      | 40      | 0            |
| 7   | T     | 738   | 0        | 404      | 61      | 0            |
| All | All   | 28928 | 0        | 27563    | 994     | 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 18.

All (994) 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) |
|------------------|------------------|--------------------------|-------------------|
| 5:M:226:LEU:CD1  | 5:M:235:LEU:HB2  | 1.31                     | 1.57              |
| 5:M:144:ILE:CD1  | 5:M:161:ILE:HG21 | 1.42                     | 1.45              |
| 5:M:226:LEU:HD12 | 5:M:235:LEU:CB   | 1.50                     | 1.39              |
| 5:M:17:PRO:HB3   | 6:N:-12:DA:C2    | 1.57                     | 1.36              |
| 5:M:23:ILE:HG21  | 7:T:12:DT:C6     | 1.66                     | 1.29              |
| 5:M:366:VAL:CG1  | 6:N:-18:DT:H3'   | 1.64                     | 1.26              |
| 5:M:16:THR:CG2   | 5:M:19:LEU:HD12  | 1.69                     | 1.23              |
| 2:C:1043:ALA:HB1 | 2:C:1044:PRO:CD  | 1.68                     | 1.22              |
| 5:M:16:THR:HG21  | 5:M:19:LEU:CB    | 1.70                     | 1.21              |
| 5:M:144:ILE:HD11 | 5:M:161:ILE:CG2  | 1.71                     | 1.19              |
| 5:M:16:THR:HG21  | 5:M:19:LEU:CD1   | 1.78                     | 1.14              |
| 5:M:144:ILE:HD11 | 5:M:161:ILE:HD13 | 1.29                     | 1.13              |
| 5:M:144:ILE:CD1  | 5:M:161:ILE:HD13 | 1.77                     | 1.13              |
| 2:C:906:PHE:CZ   | 5:M:258:PRO:HG3  | 1.83                     | 1.12              |
| 5:M:23:ILE:HG23  | 7:T:12:DT:H71    | 1.23                     | 1.12              |
| 5:M:366:VAL:HG13 | 6:N:-18:DT:H3'   | 1.13                     | 1.11              |
| 5:M:47:LEU:HD11  | 5:M:297:LEU:HD12 | 1.22                     | 1.11              |
| 5:M:16:THR:CG2   | 5:M:19:LEU:CD1   | 2.29                     | 1.10              |
| 5:M:144:ILE:CD1  | 5:M:161:ILE:CG2  | 2.25                     | 1.09              |
| 5:M:16:THR:HG21  | 5:M:19:LEU:HB3   | 1.12                     | 1.09              |
| 2:C:854:ILE:HG22 | 2:C:855:PRO:CD   | 1.82                     | 1.08              |
| 5:M:438:SER:O    | 5:M:442:LEU:HG   | 1.49                     | 1.08              |
| 5:M:278:VAL:CG1  | 5:M:392:SER:HA   | 1.83                     | 1.08              |
| 5:M:186:ASP:HB3  | 5:M:187:PRO:HD3  | 1.25                     | 1.08              |
| 5:M:421:ARG:HG3  | 5:M:465:LEU:HD11 | 1.21                     | 1.07              |
| 5:M:16:THR:CG2   | 5:M:19:LEU:HB3   | 1.84                     | 1.07              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:M:287:VAL:CG1  | 5:M:342:ARG:HA   | 1.84                     | 1.06              |
| 5:M:154:LEU:HD11 | 5:M:193:LYS:HB2  | 1.34                     | 1.05              |
| 5:M:278:VAL:HG13 | 5:M:392:SER:HA   | 1.39                     | 1.05              |
| 5:M:17:PRO:CB    | 6:N:-12:DA:C2    | 2.39                     | 1.05              |
| 2:C:854:ILE:HD12 | 2:C:854:ILE:H    | 1.22                     | 1.04              |
| 7:T:12:DT:H5''   | 7:T:13:DG:H5'    | 1.37                     | 1.04              |
| 5:M:184:ARG:NH2  | 5:M:201:ILE:HD13 | 1.72                     | 1.04              |
| 5:M:27:GLN:HB3   | 5:M:383:ARG:HG2  | 1.34                     | 1.04              |
| 5:M:125:MET:HE1  | 5:M:142:THR:HG22 | 1.35                     | 1.03              |
| 2:C:1043:ALA:HB1 | 2:C:1044:PRO:HD3 | 1.07                     | 1.02              |
| 5:M:16:THR:HG22  | 5:M:19:LEU:HD12  | 1.38                     | 1.02              |
| 5:M:144:ILE:CG1  | 5:M:161:ILE:HD13 | 1.89                     | 1.01              |
| 5:M:26:LEU:CB    | 5:M:336:ARG:CD   | 2.37                     | 1.01              |
| 5:M:469:PRO:HG3  | 6:N:-26:DG:OP1   | 1.60                     | 1.01              |
| 5:M:366:VAL:HG13 | 6:N:-17:DT:OP2   | 1.61                     | 1.01              |
| 5:M:23:ILE:HG21  | 7:T:12:DT:H6     | 1.04                     | 1.00              |
| 5:M:26:LEU:HB2   | 5:M:336:ARG:CD   | 1.91                     | 1.00              |
| 5:M:287:VAL:HG13 | 5:M:342:ARG:HA   | 1.05                     | 1.00              |
| 5:M:418:THR:HG22 | 5:M:421:ARG:HH21 | 1.22                     | 1.00              |
| 2:C:1043:ALA:CB  | 2:C:1044:PRO:CD  | 2.38                     | 0.99              |
| 2:C:854:ILE:CG2  | 2:C:855:PRO:HD2  | 1.91                     | 0.99              |
| 5:M:23:ILE:CG2   | 7:T:12:DT:C6     | 2.46                     | 0.99              |
| 6:N:-9:DA:H1'    | 6:N:-8:DT:H5'    | 1.45                     | 0.98              |
| 5:M:391:HIS:HB2  | 5:M:396:ILE:CG1  | 1.93                     | 0.98              |
| 5:M:217:ARG:HH21 | 5:M:217:ARG:HB2  | 1.29                     | 0.98              |
| 2:C:955:GLN:HE21 | 2:C:955:GLN:HA   | 1.25                     | 0.97              |
| 5:M:16:THR:HG21  | 5:M:19:LEU:HD12  | 1.38                     | 0.97              |
| 5:M:275:ASP:HB2  | 5:M:389:TYR:O    | 1.64                     | 0.97              |
| 5:M:20:GLN:C     | 5:M:23:ILE:HD11  | 1.88                     | 0.97              |
| 5:M:162:VAL:HG21 | 5:M:172:LEU:HD22 | 1.44                     | 0.97              |
| 5:M:340:LEU:HB2  | 5:M:384:VAL:HG13 | 1.47                     | 0.96              |
| 2:C:936:ARG:HD3  | 5:M:393:PRO:O    | 1.64                     | 0.96              |
| 5:M:390:LEU:O    | 5:M:396:ILE:HG23 | 1.65                     | 0.96              |
| 2:C:906:PHE:CE1  | 5:M:258:PRO:HG3  | 1.99                     | 0.96              |
| 2:C:838:CYS:HB3  | 2:C:918:LEU:HD22 | 1.48                     | 0.95              |
| 5:M:26:LEU:HB3   | 5:M:336:ARG:CG   | 1.97                     | 0.95              |
| 5:M:17:PRO:HB3   | 6:N:-12:DA:N1    | 1.81                     | 0.94              |
| 2:C:854:ILE:HG22 | 2:C:855:PRO:HD2  | 0.97                     | 0.94              |
| 5:M:26:LEU:HB3   | 5:M:336:ARG:HG3  | 1.46                     | 0.94              |
| 5:M:16:THR:HG21  | 5:M:19:LEU:CG    | 1.98                     | 0.93              |
| 5:M:386:THR:HG23 | 5:M:400:LYS:NZ   | 1.83                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:M:184:ARG:NH2  | 5:M:201:ILE:CD1  | 2.31                     | 0.93              |
| 5:M:195:LEU:CD1  | 5:M:199:LEU:HD11 | 1.98                     | 0.93              |
| 5:M:391:HIS:HA   | 5:M:396:ILE:HG13 | 1.47                     | 0.93              |
| 2:C:836:LEU:H    | 2:C:836:LEU:HD22 | 1.33                     | 0.92              |
| 5:M:16:THR:HG23  | 5:M:20:GLN:N     | 1.83                     | 0.92              |
| 5:M:144:ILE:HG21 | 5:M:179:LEU:HD23 | 1.49                     | 0.92              |
| 5:M:421:ARG:CG   | 5:M:465:LEU:HD11 | 2.00                     | 0.92              |
| 2:C:906:PHE:CZ   | 5:M:258:PRO:CG   | 2.52                     | 0.91              |
| 5:M:28:LEU:HD12  | 5:M:28:LEU:H     | 1.35                     | 0.91              |
| 5:M:456:ARG:HD3  | 7:T:24:DG:N7     | 1.85                     | 0.91              |
| 5:M:391:HIS:HB2  | 5:M:396:ILE:HG12 | 1.52                     | 0.91              |
| 5:M:366:VAL:HG13 | 6:N:-18:DT:C3'   | 1.98                     | 0.91              |
| 5:M:23:ILE:CG2   | 7:T:12:DT:H71    | 2.01                     | 0.91              |
| 5:M:46:LEU:O     | 5:M:299:ILE:HD12 | 1.70                     | 0.91              |
| 5:M:16:THR:O     | 5:M:20:GLN:HB2   | 1.71                     | 0.90              |
| 5:M:386:THR:HG23 | 5:M:400:LYS:HZ3  | 1.34                     | 0.90              |
| 5:M:349:GLU:HA   | 5:M:352:GLN:OE1  | 1.72                     | 0.90              |
| 5:M:186:ASP:HB3  | 5:M:187:PRO:CD   | 2.00                     | 0.90              |
| 5:M:20:GLN:O     | 5:M:23:ILE:CD1   | 2.20                     | 0.89              |
| 5:M:278:VAL:HG21 | 5:M:393:PRO:CD   | 2.01                     | 0.89              |
| 5:M:226:LEU:CD1  | 5:M:235:LEU:CB   | 2.26                     | 0.89              |
| 5:M:278:VAL:HG21 | 5:M:393:PRO:HD3  | 1.52                     | 0.89              |
| 5:M:140:ILE:HG22 | 5:M:178:VAL:HG11 | 1.53                     | 0.89              |
| 2:C:835:GLU:HB2  | 2:C:1053:TYR:HA  | 1.55                     | 0.88              |
| 5:M:26:LEU:CB    | 5:M:336:ARG:HD3  | 2.04                     | 0.88              |
| 2:C:1306:LYS:HD2 | 5:M:129:GLU:OE1  | 1.74                     | 0.88              |
| 5:M:23:ILE:HD12  | 5:M:23:ILE:H     | 1.38                     | 0.88              |
| 5:M:297:LEU:O    | 5:M:330:ILE:HD12 | 1.71                     | 0.87              |
| 5:M:456:ARG:HH11 | 7:T:24:DG:H8     | 1.22                     | 0.87              |
| 5:M:144:ILE:HD11 | 5:M:161:ILE:CD1  | 2.04                     | 0.87              |
| 5:M:144:ILE:HD11 | 5:M:161:ILE:HG21 | 0.87                     | 0.87              |
| 2:C:871:VAL:HG21 | 2:C:883:LEU:HD12 | 1.54                     | 0.87              |
| 2:C:902:LEU:HD23 | 2:C:910:ALA:CB   | 2.05                     | 0.87              |
| 5:M:181:ARG:O    | 5:M:181:ARG:HD3  | 1.74                     | 0.87              |
| 5:M:386:THR:CG2  | 5:M:400:LYS:NZ   | 2.38                     | 0.87              |
| 5:M:26:LEU:HB2   | 5:M:336:ARG:HD2  | 1.54                     | 0.86              |
| 5:M:400:LYS:HE3  | 6:N:-16:DT:OP2   | 1.75                     | 0.86              |
| 5:M:20:GLN:O     | 5:M:23:ILE:HD11  | 1.75                     | 0.86              |
| 5:M:287:VAL:HG13 | 5:M:342:ARG:CA   | 2.00                     | 0.86              |
| 6:N:-10:DG:H1    | 7:T:10:DC:H42    | 1.19                     | 0.86              |
| 5:M:39:GLN:O     | 5:M:39:GLN:NE2   | 2.08                     | 0.86              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:M:26:LEU:HD13   | 5:M:26:LEU:H     | 1.41                     | 0.86              |
| 5:M:49:GLU:HA     | 5:M:296:ARG:O    | 1.75                     | 0.86              |
| 5:M:279:ARG:NH2   | 5:M:279:ARG:O    | 2.09                     | 0.85              |
| 5:M:277:LEU:HD12  | 5:M:277:LEU:H    | 1.40                     | 0.85              |
| 1:A:315:GLY:HA3   | 5:M:132:PRO:HG3  | 1.58                     | 0.85              |
| 5:M:26:LEU:HB3    | 5:M:336:ARG:CD   | 2.04                     | 0.85              |
| 6:N:-11:DC:H42    | 7:T:11:DG:H1     | 1.24                     | 0.84              |
| 5:M:366:VAL:HG11  | 6:N:-18:DT:H3'   | 1.57                     | 0.84              |
| 5:M:431:GLU:OE1   | 5:M:437:LEU:HG   | 1.76                     | 0.84              |
| 2:C:1022:LYS:HA   | 2:C:1022:LYS:CE  | 2.07                     | 0.83              |
| 5:M:400:LYS:HE3   | 6:N:-16:DT:P     | 2.18                     | 0.83              |
| 5:M:278:VAL:CG2   | 5:M:393:PRO:HD3  | 2.08                     | 0.83              |
| 2:C:1042:LEU:HD12 | 2:C:1042:LEU:H   | 1.43                     | 0.83              |
| 5:M:297:LEU:HB3   | 5:M:330:ILE:CD1  | 2.09                     | 0.83              |
| 5:M:456:ARG:NH1   | 7:T:24:DG:C8     | 2.46                     | 0.83              |
| 5:M:123:TYR:CZ    | 5:M:186:ASP:OD2  | 2.32                     | 0.83              |
| 5:M:217:ARG:HB2   | 5:M:217:ARG:NH2  | 1.95                     | 0.82              |
| 2:C:1032:LYS:O    | 2:C:1032:LYS:HD3 | 1.79                     | 0.82              |
| 2:C:964:LEU:O     | 2:C:964:LEU:HD12 | 1.80                     | 0.82              |
| 2:C:1254:VAL:HG21 | 5:M:112:TYR:CB   | 2.10                     | 0.82              |
| 5:M:280:LYS:HE2   | 5:M:280:LYS:O    | 1.80                     | 0.81              |
| 5:M:197:ASP:OD1   | 5:M:197:ASP:N    | 2.14                     | 0.81              |
| 5:M:336:ARG:C     | 5:M:336:ARG:HE   | 1.89                     | 0.81              |
| 5:M:294:ILE:HD12  | 5:M:295:PRO:HD2  | 1.62                     | 0.81              |
| 2:C:974:ARG:HH21  | 2:C:974:ARG:HB2  | 1.42                     | 0.80              |
| 2:C:1011:LEU:HD22 | 2:C:1011:LEU:O   | 1.81                     | 0.80              |
| 5:M:144:ILE:HG13  | 5:M:161:ILE:HD13 | 1.61                     | 0.80              |
| 5:M:259:ARG:HG3   | 5:M:259:ARG:HH11 | 1.45                     | 0.80              |
| 5:M:17:PRO:HG3    | 6:N:-12:DA:C4    | 2.17                     | 0.80              |
| 5:M:193:LYS:HD2   | 5:M:193:LYS:O    | 1.81                     | 0.80              |
| 6:N:-13:DC:H42    | 7:T:13:DG:H1     | 1.29                     | 0.80              |
| 2:C:1032:LYS:CE   | 2:C:1032:LYS:HA  | 2.11                     | 0.80              |
| 5:M:386:THR:HG22  | 5:M:400:LYS:HE2  | 1.64                     | 0.79              |
| 5:M:349:GLU:O     | 5:M:352:GLN:HG2  | 1.82                     | 0.79              |
| 5:M:391:HIS:CA    | 5:M:396:ILE:HG13 | 2.11                     | 0.79              |
| 2:C:1032:LYS:HA   | 2:C:1032:LYS:HZ2 | 1.45                     | 0.79              |
| 5:M:400:LYS:CE    | 6:N:-16:DT:OP2   | 2.30                     | 0.79              |
| 5:M:22:ALA:HA     | 5:M:25:LEU:HD13  | 1.65                     | 0.78              |
| 5:M:15:MET:CE     | 6:N:-11:DC:H5''  | 2.13                     | 0.78              |
| 5:M:20:GLN:C      | 5:M:23:ILE:CD1   | 2.57                     | 0.78              |
| 5:M:154:LEU:CD1   | 5:M:193:LYS:HB2  | 2.11                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:M:278:VAL:HG11 | 5:M:392:SER:CB   | 2.13                     | 0.78              |
| 5:M:19:LEU:O     | 5:M:19:LEU:HD22  | 1.84                     | 0.78              |
| 5:M:386:THR:CG2  | 5:M:400:LYS:CE   | 2.62                     | 0.78              |
| 5:M:287:VAL:HG21 | 5:M:345:ARG:NH1  | 1.99                     | 0.77              |
| 5:M:456:ARG:HD2  | 7:T:23:DT:H2'    | 1.65                     | 0.77              |
| 5:M:16:THR:HG23  | 5:M:20:GLN:H     | 1.47                     | 0.77              |
| 2:C:992:LEU:HD22 | 2:C:993:PRO:HD2  | 1.66                     | 0.77              |
| 5:M:26:LEU:CB    | 5:M:336:ARG:CG   | 2.63                     | 0.77              |
| 7:T:9:DT:H2''    | 7:T:10:DC:H5''   | 1.67                     | 0.77              |
| 5:M:278:VAL:CG1  | 5:M:392:SER:CB   | 2.63                     | 0.77              |
| 5:M:278:VAL:HG11 | 5:M:392:SER:HA   | 1.65                     | 0.77              |
| 5:M:456:ARG:HG3  | 7:T:23:DT:C5     | 2.20                     | 0.77              |
| 2:C:906:PHE:CE1  | 5:M:258:PRO:CG   | 2.68                     | 0.77              |
| 5:M:26:LEU:HB2   | 5:M:336:ARG:HD3  | 1.64                     | 0.77              |
| 1:A:68:TYR:HB3   | 2:C:929:ILE:CD1  | 2.15                     | 0.76              |
| 5:M:456:ARG:NH1  | 7:T:24:DG:H8     | 1.82                     | 0.76              |
| 5:M:19:LEU:O     | 5:M:23:ILE:HG13  | 1.84                     | 0.76              |
| 5:M:278:VAL:CG1  | 5:M:392:SER:CA   | 2.61                     | 0.76              |
| 2:C:953:LEU:HD12 | 2:C:953:LEU:O    | 1.84                     | 0.76              |
| 5:M:295:PRO:HD2  | 5:M:333:LEU:HD21 | 1.66                     | 0.76              |
| 2:C:955:GLN:HA   | 2:C:955:GLN:NE2  | 1.96                     | 0.76              |
| 5:M:456:ARG:HD2  | 7:T:23:DT:C2'    | 2.16                     | 0.76              |
| 5:M:144:ILE:HD13 | 5:M:161:ILE:HG21 | 1.61                     | 0.76              |
| 5:M:294:ILE:HD12 | 5:M:295:PRO:CD   | 2.16                     | 0.76              |
| 2:C:1022:LYS:HA  | 2:C:1022:LYS:HZ3 | 1.50                     | 0.76              |
| 5:M:225:ASP:OD1  | 5:M:225:ASP:N    | 2.17                     | 0.76              |
| 5:M:217:ARG:HH21 | 5:M:217:ARG:CB   | 1.99                     | 0.75              |
| 5:M:391:HIS:HB2  | 5:M:396:ILE:HG13 | 1.67                     | 0.75              |
| 5:M:277:LEU:HD12 | 5:M:277:LEU:N    | 2.01                     | 0.75              |
| 2:C:902:LEU:HD23 | 2:C:910:ALA:HB1  | 1.68                     | 0.75              |
| 5:M:180:LYS:HZ3  | 5:M:180:LYS:C    | 1.95                     | 0.75              |
| 5:M:340:LEU:HB2  | 5:M:384:VAL:CG1  | 2.17                     | 0.75              |
| 5:M:46:LEU:O     | 5:M:299:ILE:CD1  | 2.34                     | 0.74              |
| 5:M:184:ARG:HH11 | 5:M:205:GLN:HE22 | 1.35                     | 0.74              |
| 5:M:27:GLN:CB    | 5:M:383:ARG:HG2  | 2.16                     | 0.74              |
| 5:M:16:THR:CG2   | 5:M:19:LEU:CB    | 2.55                     | 0.74              |
| 5:M:421:ARG:HG3  | 5:M:465:LEU:CD1  | 2.10                     | 0.74              |
| 5:M:273:ILE:H    | 5:M:273:ILE:HD12 | 1.53                     | 0.74              |
| 5:M:47:LEU:CD1   | 5:M:297:LEU:HD12 | 2.11                     | 0.73              |
| 2:C:979:LEU:C    | 2:C:979:LEU:HD12 | 2.14                     | 0.73              |
| 5:M:278:VAL:HG11 | 5:M:392:SER:HB2  | 1.69                     | 0.73              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:M:227:LEU:HD13  | 5:M:227:LEU:C    | 2.14                     | 0.73              |
| 2:C:1032:LYS:HA   | 2:C:1032:LYS:NZ  | 2.04                     | 0.73              |
| 5:M:226:LEU:HD12  | 5:M:235:LEU:HB2  | 0.73                     | 0.73              |
| 2:C:1043:ALA:CB   | 2:C:1044:PRO:HD3 | 1.96                     | 0.73              |
| 5:M:26:LEU:HB3    | 5:M:336:ARG:HD3  | 1.69                     | 0.73              |
| 5:M:150:ASP:N     | 5:M:150:ASP:OD1  | 2.22                     | 0.73              |
| 5:M:456:ARG:HG3   | 7:T:23:DT:H73    | 1.70                     | 0.73              |
| 7:T:33:DC:H2"     | 7:T:34:DT:C6     | 2.24                     | 0.73              |
| 5:M:226:LEU:HD13  | 5:M:235:LEU:HB2  | 1.62                     | 0.72              |
| 5:M:289:LEU:C     | 5:M:289:LEU:HD23 | 2.15                     | 0.72              |
| 5:M:19:LEU:HD13   | 5:M:19:LEU:C     | 2.15                     | 0.72              |
| 1:A:312:LEU:HD22  | 5:M:181:ARG:NH1  | 2.03                     | 0.72              |
| 5:M:340:LEU:CD1   | 5:M:388:LYS:HD2  | 2.20                     | 0.72              |
| 2:C:1022:LYS:HZ3  | 2:C:1022:LYS:CA  | 2.02                     | 0.72              |
| 5:M:400:LYS:NZ    | 6:N:-16:DT:OP2   | 2.22                     | 0.72              |
| 7:T:32:DT:H2"     | 7:T:33:DC:C5     | 2.25                     | 0.72              |
| 1:A:45:ARG:NH1    | 1:B:38:THR:OG1   | 2.22                     | 0.71              |
| 5:M:121:GLN:OE1   | 5:M:121:GLN:HA   | 1.90                     | 0.71              |
| 5:M:343:VAL:HG11  | 5:M:384:VAL:HG11 | 1.70                     | 0.71              |
| 5:M:456:ARG:HH11  | 7:T:23:DT:H2"    | 1.55                     | 0.71              |
| 2:C:918:LEU:C     | 2:C:918:LEU:HD12 | 2.15                     | 0.71              |
| 5:M:339:THR:O     | 5:M:343:VAL:HB   | 1.90                     | 0.71              |
| 2:C:856:ASN:ND2   | 5:M:257:ASP:OD2  | 2.23                     | 0.71              |
| 2:C:1032:LYS:HD3  | 2:C:1032:LYS:C   | 2.15                     | 0.71              |
| 3:D:43:THR:HG22   | 3:D:56:LEU:HB2   | 1.73                     | 0.71              |
| 5:M:179:LEU:HD22  | 5:M:179:LEU:O    | 1.90                     | 0.71              |
| 2:C:1032:LYS:HZ2  | 2:C:1032:LYS:CA  | 2.03                     | 0.71              |
| 2:C:1029:LEU:HD12 | 2:C:1029:LEU:O   | 1.91                     | 0.71              |
| 5:M:138:ARG:HB2   | 5:M:138:ARG:CZ   | 2.21                     | 0.71              |
| 5:M:184:ARG:HH21  | 5:M:201:ILE:CD1  | 2.03                     | 0.71              |
| 1:A:11:PRO:HA     | 1:A:30:PRO:HG2   | 1.73                     | 0.70              |
| 5:M:140:ILE:HG12  | 5:M:165:ILE:HD13 | 1.72                     | 0.70              |
| 5:M:130:LEU:HD23  | 5:M:130:LEU:N    | 2.05                     | 0.70              |
| 5:M:297:LEU:O     | 5:M:330:ILE:CD1  | 2.38                     | 0.70              |
| 5:M:456:ARG:HG3   | 7:T:23:DT:C7     | 2.21                     | 0.70              |
| 2:C:960:LEU:C     | 2:C:960:LEU:HD12 | 2.17                     | 0.70              |
| 5:M:16:THR:O      | 5:M:20:GLN:CB    | 2.38                     | 0.70              |
| 5:M:23:ILE:HD12   | 5:M:23:ILE:N     | 2.03                     | 0.70              |
| 5:M:390:LEU:HB3   | 5:M:399:LEU:HD21 | 1.73                     | 0.70              |
| 5:M:125:MET:HE1   | 5:M:142:THR:CG2  | 2.19                     | 0.70              |
| 5:M:388:LYS:O     | 5:M:399:LEU:HD23 | 1.92                     | 0.70              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:1011:LEU:HD22 | 2:C:1011:LEU:C   | 2.14                     | 0.70              |
| 5:M:15:MET:HE1    | 6:N:-11:DC:H5''  | 1.72                     | 0.69              |
| 5:M:366:VAL:CG1   | 6:N:-17:DT:OP2   | 2.39                     | 0.69              |
| 1:B:46:ILE:HG13   | 1:B:224:LEU:HG   | 1.73                     | 0.69              |
| 2:C:953:LEU:HD12  | 2:C:953:LEU:C    | 2.17                     | 0.69              |
| 5:M:421:ARG:HD2   | 5:M:465:LEU:HD21 | 1.74                     | 0.69              |
| 2:C:1022:LYS:HA   | 2:C:1022:LYS:NZ  | 2.06                     | 0.69              |
| 5:M:366:VAL:HG21  | 6:N:-18:DT:H5''  | 1.73                     | 0.69              |
| 5:M:456:ARG:HG3   | 7:T:23:DT:C6     | 2.28                     | 0.69              |
| 5:M:140:ILE:HG12  | 5:M:165:ILE:CD1  | 2.23                     | 0.69              |
| 5:M:273:ILE:HD12  | 5:M:273:ILE:N    | 2.07                     | 0.69              |
| 5:M:278:VAL:HG11  | 5:M:393:PRO:CD   | 2.23                     | 0.69              |
| 5:M:391:HIS:CB    | 5:M:396:ILE:HG13 | 2.23                     | 0.69              |
| 5:M:23:ILE:HG23   | 7:T:12:DT:C7     | 2.13                     | 0.69              |
| 5:M:336:ARG:HH21  | 5:M:337:ASN:HA   | 1.57                     | 0.69              |
| 5:M:181:ARG:HD3   | 5:M:181:ARG:C    | 2.16                     | 0.68              |
| 5:M:41:LEU:HG     | 5:M:41:LEU:O     | 1.92                     | 0.68              |
| 2:C:987:GLU:H     | 2:C:987:GLU:CD   | 2.01                     | 0.68              |
| 5:M:140:ILE:CG2   | 5:M:178:VAL:HG11 | 2.24                     | 0.68              |
| 5:M:226:LEU:HD12  | 5:M:235:LEU:CG   | 2.23                     | 0.68              |
| 5:M:438:SER:OG    | 5:M:439:ASP:N    | 2.27                     | 0.68              |
| 5:M:295:PRO:O     | 5:M:297:LEU:HD23 | 1.94                     | 0.68              |
| 5:M:28:LEU:CD2    | 5:M:32:GLU:HB3   | 2.24                     | 0.67              |
| 2:C:213:LEU:O     | 2:C:214:ASN:ND2  | 2.27                     | 0.67              |
| 5:M:127:GLN:HE22  | 5:M:186:ASP:N    | 1.93                     | 0.67              |
| 5:M:278:VAL:HG11  | 5:M:392:SER:CA   | 2.23                     | 0.67              |
| 1:A:312:LEU:HB3   | 5:M:181:ARG:HH11 | 1.59                     | 0.67              |
| 2:C:979:LEU:HD12  | 2:C:979:LEU:O    | 1.95                     | 0.67              |
| 2:C:1253:LEU:HG   | 5:M:114:GLY:O    | 1.95                     | 0.67              |
| 2:C:932:GLN:HA    | 2:C:932:GLN:NE2  | 2.09                     | 0.67              |
| 5:M:386:THR:CG2   | 5:M:400:LYS:HE2  | 2.24                     | 0.67              |
| 5:M:376:MET:HE3   | 5:M:380:THR:HG21 | 1.75                     | 0.67              |
| 5:M:349:GLU:HG2   | 5:M:352:GLN:OE1  | 1.94                     | 0.66              |
| 5:M:421:ARG:CD    | 5:M:465:LEU:HD21 | 2.25                     | 0.66              |
| 2:C:700:VAL:HG21  | 2:C:1114:GLU:HG3 | 1.78                     | 0.66              |
| 5:M:187:PRO:HG2   | 5:M:190:VAL:HB   | 1.76                     | 0.66              |
| 5:M:295:PRO:O     | 5:M:297:LEU:CD2  | 2.43                     | 0.66              |
| 5:M:26:LEU:HG     | 5:M:336:ARG:HG2  | 1.78                     | 0.66              |
| 5:M:195:LEU:CG    | 5:M:199:LEU:HD11 | 2.26                     | 0.66              |
| 2:C:836:LEU:HD22  | 2:C:836:LEU:N    | 2.02                     | 0.66              |
| 5:M:406:HIS:CE1   | 7:T:22:DG:H4'    | 2.31                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:287:VAL:HG21  | 5:M:345:ARG:HH12  | 1.59                     | 0.66              |
| 5:M:405:SER:OG    | 7:T:21:DC:H5'     | 1.96                     | 0.65              |
| 3:D:920:ALA:HB2   | 3:D:1256:ILE:HD11 | 1.78                     | 0.65              |
| 2:C:906:PHE:CZ    | 5:M:258:PRO:CD    | 2.79                     | 0.65              |
| 3:D:425:ARG:HG2   | 3:D:427:PRO:HD2   | 1.78                     | 0.65              |
| 3:D:45:ASN:ND2    | 3:D:50:LYS:O      | 2.30                     | 0.65              |
| 1:A:68:TYR:HB3    | 2:C:929:ILE:HD13  | 1.78                     | 0.65              |
| 5:M:20:GLN:CA     | 5:M:23:ILE:HD11   | 2.26                     | 0.65              |
| 5:M:124:LEU:HD12  | 5:M:145:VAL:HG21  | 1.79                     | 0.65              |
| 1:B:47:LEU:HD13   | 1:B:220:ALA:HB2   | 1.78                     | 0.65              |
| 5:M:28:LEU:C      | 5:M:28:LEU:HD13   | 2.22                     | 0.65              |
| 2:C:954:LYS:HD2   | 2:C:954:LYS:O     | 1.96                     | 0.65              |
| 3:D:803:VAL:HG22  | 3:D:1313:SER:HB3  | 1.78                     | 0.65              |
| 5:M:173:GLU:OE1   | 5:M:173:GLU:N     | 2.29                     | 0.65              |
| 3:D:98:ARG:HG2    | 3:D:248:ASP:HB2   | 1.79                     | 0.64              |
| 5:M:120:LEU:HD13  | 5:M:120:LEU:O     | 1.97                     | 0.64              |
| 2:C:1101:LEU:HD13 | 3:D:725:MET:HE3   | 1.79                     | 0.64              |
| 5:M:20:GLN:O      | 5:M:20:GLN:NE2    | 2.29                     | 0.64              |
| 5:M:120:LEU:O     | 5:M:120:LEU:HD22  | 1.97                     | 0.64              |
| 5:M:172:LEU:N     | 5:M:172:LEU:HD23  | 2.11                     | 0.64              |
| 5:M:23:ILE:CG2    | 7:T:12:DT:C5      | 2.79                     | 0.64              |
| 5:M:195:LEU:O     | 5:M:199:LEU:HD12  | 1.98                     | 0.64              |
| 5:M:287:VAL:CG1   | 5:M:342:ARG:CA    | 2.71                     | 0.64              |
| 2:C:974:ARG:HH21  | 2:C:974:ARG:CB    | 2.11                     | 0.64              |
| 5:M:186:ASP:CB    | 5:M:187:PRO:HD3   | 2.17                     | 0.64              |
| 5:M:195:LEU:HD11  | 5:M:199:LEU:HD11  | 1.80                     | 0.64              |
| 5:M:384:VAL:O     | 5:M:388:LYS:HG3   | 1.97                     | 0.64              |
| 1:A:45:ARG:NH2    | 2:C:1084:ASP:OD1  | 2.31                     | 0.64              |
| 5:M:17:PRO:C      | 5:M:19:LEU:H      | 2.05                     | 0.64              |
| 5:M:347:ILE:HG13  | 5:M:365:MET:HE1   | 1.80                     | 0.64              |
| 5:M:376:MET:CE    | 5:M:380:THR:HG21  | 2.27                     | 0.64              |
| 2:C:817:LEU:HB3   | 2:C:1097:VAL:HB   | 1.80                     | 0.63              |
| 2:C:848:GLU:OE1   | 2:C:848:GLU:N     | 2.30                     | 0.63              |
| 5:M:297:LEU:HB3   | 5:M:330:ILE:HD13  | 1.79                     | 0.63              |
| 1:A:68:TYR:CB     | 2:C:929:ILE:HD13  | 2.28                     | 0.63              |
| 1:A:315:GLY:HA3   | 5:M:132:PRO:CG    | 2.26                     | 0.63              |
| 1:B:74:VAL:HG13   | 1:B:76:GLU:H      | 1.62                     | 0.63              |
| 2:C:918:LEU:HD12  | 2:C:918:LEU:O     | 1.98                     | 0.63              |
| 2:C:802:VAL:HG21  | 2:C:1230:MET:HE3  | 1.79                     | 0.63              |
| 2:C:706:ARG:NH2   | 2:C:791:LEU:O     | 2.32                     | 0.63              |
| 5:M:390:LEU:HD22  | 5:M:397:PHE:H     | 1.63                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:M:455:ARG:NH2  | 6:N:-26:DG:O6     | 2.27                     | 0.63              |
| 2:C:1070:HIS:NE2 | 2:C:1114:GLU:OE1  | 2.32                     | 0.63              |
| 5:M:154:LEU:HD12 | 5:M:154:LEU:O     | 1.98                     | 0.63              |
| 5:M:195:LEU:HG   | 5:M:199:LEU:HD11  | 1.78                     | 0.63              |
| 5:M:366:VAL:HG12 | 5:M:368:ALA:H     | 1.64                     | 0.63              |
| 5:M:289:LEU:HD23 | 5:M:289:LEU:O     | 1.98                     | 0.63              |
| 2:C:854:ILE:CG2  | 2:C:855:PRO:CD    | 2.64                     | 0.63              |
| 5:M:15:MET:HE3   | 6:N:-11:DC:H5"    | 1.79                     | 0.63              |
| 1:B:97:GLU:OE2   | 1:B:145:LYS:NZ    | 2.31                     | 0.62              |
| 2:C:229:ILE:HD12 | 2:C:240:GLU:H     | 1.63                     | 0.62              |
| 2:C:490:GLN:O    | 2:C:490:GLN:NE2   | 2.33                     | 0.62              |
| 3:D:1145:PHE:HB3 | 3:D:1309:ILE:HD12 | 1.81                     | 0.62              |
| 5:M:16:THR:HG22  | 5:M:19:LEU:CD1    | 2.14                     | 0.62              |
| 2:C:987:GLU:OE1  | 2:C:987:GLU:N     | 2.19                     | 0.62              |
| 5:M:23:ILE:CG2   | 7:T:12:DT:C7      | 2.74                     | 0.62              |
| 5:M:21:GLN:C     | 5:M:23:ILE:H      | 2.07                     | 0.62              |
| 5:M:144:ILE:HD12 | 5:M:161:ILE:CG2   | 2.28                     | 0.62              |
| 5:M:347:ILE:HD11 | 5:M:402:PHE:HD2   | 1.64                     | 0.62              |
| 2:C:949:GLU:HA   | 2:C:949:GLU:OE1   | 2.00                     | 0.62              |
| 5:M:125:MET:CE   | 5:M:142:THR:HG22  | 2.22                     | 0.62              |
| 5:M:179:LEU:O    | 5:M:179:LEU:HD13  | 1.99                     | 0.62              |
| 5:M:386:THR:HG22 | 5:M:400:LYS:HG3   | 1.81                     | 0.62              |
| 2:C:808:ASN:H    | 3:D:633:ALA:HB2   | 1.65                     | 0.62              |
| 1:B:41:ASN:OD1   | 1:B:44:ARG:NH1    | 2.33                     | 0.62              |
| 1:B:29:GLU:HG3   | 1:B:30:PRO:HD2    | 1.82                     | 0.62              |
| 2:C:804:PHE:HB3  | 2:C:1100:PRO:HB3  | 1.82                     | 0.62              |
| 3:D:819:GLY:HA2  | 3:D:883:ARG:HA    | 1.82                     | 0.62              |
| 5:M:17:PRO:O     | 5:M:19:LEU:N      | 2.32                     | 0.62              |
| 5:M:345:ARG:HG2  | 5:M:345:ARG:O     | 1.99                     | 0.62              |
| 5:M:386:THR:HG22 | 5:M:400:LYS:CE    | 2.28                     | 0.62              |
| 3:D:1268:ASN:HB3 | 3:D:1300:ALA:HA   | 1.82                     | 0.61              |
| 5:M:19:LEU:HD23  | 7:T:12:DT:H72     | 1.82                     | 0.61              |
| 2:C:975:ILE:HD11 | 2:C:1014:LEU:HB3  | 1.83                     | 0.61              |
| 3:D:482:ALA:HA   | 4:E:6:VAL:HG21    | 1.82                     | 0.61              |
| 5:M:144:ILE:HG13 | 5:M:161:ILE:CD1   | 2.30                     | 0.61              |
| 5:M:281:VAL:O    | 5:M:281:VAL:HG13  | 2.01                     | 0.61              |
| 5:M:366:VAL:HG13 | 6:N:-17:DT:P      | 2.40                     | 0.61              |
| 5:M:418:THR:HG22 | 5:M:421:ARG:NH2   | 2.05                     | 0.61              |
| 1:B:100:LEU:HD21 | 1:B:121:VAL:HG21  | 1.83                     | 0.61              |
| 3:D:576:ARG:NH1  | 3:D:593:ASN:OD1   | 2.33                     | 0.61              |
| 3:D:584:PRO:HG2  | 3:D:587:LEU:HD13  | 1.83                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:800:LEU:HB3   | 3:D:920:ALA:HB1   | 1.82                     | 0.61              |
| 5:M:196:ARG:HH21  | 5:M:196:ARG:CG    | 2.14                     | 0.61              |
| 5:M:262:GLN:O     | 5:M:262:GLN:HG2   | 2.00                     | 0.61              |
| 5:M:340:LEU:HD13  | 5:M:388:LYS:HD2   | 1.82                     | 0.61              |
| 2:C:954:LYS:HD2   | 2:C:954:LYS:C     | 2.25                     | 0.61              |
| 2:C:1043:ALA:HB3  | 2:C:1046:VAL:HG23 | 1.83                     | 0.61              |
| 1:A:312:LEU:HD22  | 5:M:181:ARG:HH12  | 1.66                     | 0.60              |
| 2:C:12:ARG:HG3    | 2:C:1181:PRO:HB2  | 1.82                     | 0.60              |
| 2:C:1241:ASP:O    | 2:C:1262:LYS:NZ   | 2.31                     | 0.60              |
| 7:T:12:DT:H5''    | 7:T:13:DG:C5'     | 2.24                     | 0.60              |
| 2:C:371:ARG:NH1   | 2:C:373:GLY:O     | 2.34                     | 0.60              |
| 2:C:526:HIS:CE1   | 2:C:529:ARG:HH21  | 2.18                     | 0.60              |
| 3:D:281:ARG:HG2   | 5:M:42:GLU:OE2    | 2.00                     | 0.60              |
| 3:D:1161:GLY:HA2  | 3:D:1179:PRO:HB3  | 1.82                     | 0.60              |
| 2:C:896:THR:HG23  | 2:C:896:THR:O     | 2.00                     | 0.60              |
| 5:M:294:ILE:O     | 5:M:294:ILE:HG23  | 2.01                     | 0.60              |
| 5:M:287:VAL:CG2   | 5:M:345:ARG:NH1   | 2.63                     | 0.60              |
| 1:A:101:THR:HG22  | 1:A:143:ARG:HG2   | 1.82                     | 0.60              |
| 5:M:154:LEU:HD12  | 5:M:154:LEU:C     | 2.27                     | 0.60              |
| 5:M:288:GLU:OE1   | 5:M:288:GLU:HA    | 2.02                     | 0.60              |
| 1:A:262:LEU:HG    | 1:A:267:ALA:HB2   | 1.84                     | 0.60              |
| 5:M:26:LEU:HD13   | 5:M:26:LEU:N      | 2.14                     | 0.60              |
| 5:M:37:LEU:HD11   | 5:M:297:LEU:HD21  | 1.84                     | 0.60              |
| 5:M:111:VAL:HG22  | 5:M:111:VAL:O     | 2.00                     | 0.60              |
| 5:M:226:LEU:HD11  | 5:M:235:LEU:HB2   | 1.66                     | 0.60              |
| 2:C:212:ALA:O     | 2:C:359:ARG:NH1   | 2.35                     | 0.60              |
| 2:C:1062:PRO:HA   | 2:C:1076:ILE:HB   | 1.83                     | 0.59              |
| 5:M:366:VAL:CG1   | 6:N:-18:DT:C3'    | 2.60                     | 0.59              |
| 1:A:80:GLU:O      | 1:A:84:ASN:ND2    | 2.35                     | 0.59              |
| 2:C:1050:VAL:HG22 | 2:C:1050:VAL:O    | 2.02                     | 0.59              |
| 3:D:826:ILE:HB    | 3:D:993:GLU:HA    | 1.84                     | 0.59              |
| 5:M:16:THR:HG23   | 5:M:16:THR:O      | 2.02                     | 0.59              |
| 2:C:239:MET:HE2   | 2:C:287:VAL:HG21  | 1.84                     | 0.59              |
| 2:C:884:VAL:O     | 2:C:884:VAL:HG12  | 2.01                     | 0.59              |
| 3:D:268:LEU:HD13  | 3:D:306:LEU:HA    | 1.85                     | 0.59              |
| 5:M:45:PRO:HD2    | 5:M:322:ASN:HD22  | 1.67                     | 0.59              |
| 2:C:928:VAL:HG22  | 2:C:928:VAL:O     | 2.00                     | 0.59              |
| 2:C:939:VAL:HG21  | 2:C:1047:LEU:HD11 | 1.85                     | 0.59              |
| 5:M:28:LEU:HD22   | 5:M:32:GLU:HB3    | 1.83                     | 0.59              |
| 2:C:964:LEU:HD12  | 2:C:964:LEU:C     | 2.26                     | 0.59              |
| 2:C:1339:LEU:HD23 | 3:D:20:ILE:HD13   | 1.85                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:124:VAL:HG13 | 1:B:125:LYS:HG2  | 1.85                     | 0.59              |
| 2:C:1020:GLU:HA  | 2:C:1020:GLU:OE2 | 2.03                     | 0.59              |
| 5:M:456:ARG:HG2  | 5:M:457:THR:H    | 1.67                     | 0.59              |
| 1:A:307:LEU:O    | 1:A:312:LEU:N    | 2.35                     | 0.58              |
| 2:C:211:ARG:NH1  | 2:C:356:THR:O    | 2.36                     | 0.58              |
| 5:M:193:LYS:HD2  | 5:M:193:LYS:C    | 2.28                     | 0.58              |
| 5:M:259:ARG:HG2  | 5:M:259:ARG:O    | 2.02                     | 0.58              |
| 5:M:275:ASP:CB   | 5:M:389:TYR:O    | 2.45                     | 0.58              |
| 5:M:340:LEU:HD11 | 5:M:388:LYS:HD2  | 1.84                     | 0.58              |
| 1:A:312:LEU:HB3  | 5:M:181:ARG:NH1  | 2.18                     | 0.58              |
| 3:D:676:GLY:O    | 3:D:680:ASN:ND2  | 2.33                     | 0.58              |
| 5:M:226:LEU:HD12 | 5:M:235:LEU:CA   | 2.28                     | 0.58              |
| 5:M:406:HIS:O    | 7:T:22:DG:H5"    | 2.03                     | 0.58              |
| 5:M:28:LEU:HD12  | 5:M:28:LEU:N     | 2.09                     | 0.58              |
| 5:M:184:ARG:HH21 | 5:M:201:ILE:HD11 | 1.68                     | 0.58              |
| 5:M:49:GLU:CA    | 5:M:296:ARG:O    | 2.50                     | 0.58              |
| 1:A:312:LEU:CB   | 5:M:181:ARG:HH11 | 2.17                     | 0.58              |
| 5:M:279:ARG:HB2  | 5:M:286:THR:HG22 | 1.85                     | 0.58              |
| 2:C:902:LEU:CD2  | 2:C:910:ALA:CB   | 2.81                     | 0.57              |
| 2:C:833:ILE:O    | 2:C:833:ILE:HG22 | 2.03                     | 0.57              |
| 3:D:653:ILE:HG23 | 3:D:692:ARG:HH11 | 1.69                     | 0.57              |
| 5:M:386:THR:HG23 | 5:M:400:LYS:CE   | 2.32                     | 0.57              |
| 5:M:16:THR:CG2   | 5:M:19:LEU:HD13  | 2.30                     | 0.57              |
| 5:M:438:SER:O    | 5:M:442:LEU:CG   | 2.40                     | 0.57              |
| 6:N:-7:DC:H2"    | 6:N:-6:DA:C8     | 2.39                     | 0.57              |
| 1:A:68:TYR:CB    | 2:C:929:ILE:CD1  | 2.83                     | 0.57              |
| 1:B:84:ASN:ND2   | 1:B:129:VAL:O    | 2.36                     | 0.57              |
| 2:C:197:ARG:HA   | 2:C:204:LEU:HD13 | 1.85                     | 0.57              |
| 7:T:11:DG:OP2    | 7:T:11:DG:C8     | 2.57                     | 0.57              |
| 2:C:1251:TYR:N   | 2:C:1251:TYR:CD1 | 2.73                     | 0.57              |
| 5:M:19:LEU:HD22  | 5:M:23:ILE:HG13  | 1.87                     | 0.57              |
| 5:M:28:LEU:H     | 5:M:28:LEU:CD1   | 2.13                     | 0.57              |
| 2:C:902:LEU:CD2  | 2:C:910:ALA:HB1  | 2.34                     | 0.57              |
| 5:M:47:LEU:HD11  | 5:M:297:LEU:CD1  | 2.16                     | 0.57              |
| 1:A:315:GLY:CA   | 5:M:132:PRO:HG3  | 2.34                     | 0.57              |
| 5:M:200:LEU:HD13 | 5:M:200:LEU:C    | 2.29                     | 0.57              |
| 2:C:1022:LYS:HZ3 | 2:C:1022:LYS:CB  | 2.18                     | 0.56              |
| 2:C:1043:ALA:CB  | 2:C:1044:PRO:HD2 | 2.33                     | 0.56              |
| 2:C:914:LYS:HD3  | 5:M:267:SER:OG   | 2.05                     | 0.56              |
| 2:C:960:LEU:HD21 | 2:C:1029:LEU:HB2 | 1.86                     | 0.56              |
| 2:C:1154:ASP:OD1 | 2:C:1157:GLN:NE2 | 2.38                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:906:PHE:HZ   | 5:M:258:PRO:HG3  | 1.58                     | 0.56              |
| 3:D:807:LEU:HD11 | 3:D:894:VAL:HG23 | 1.87                     | 0.56              |
| 5:M:278:VAL:HG11 | 5:M:393:PRO:HD2  | 1.88                     | 0.56              |
| 5:M:386:THR:CG2  | 5:M:400:LYS:HZ1  | 2.16                     | 0.56              |
| 5:M:19:LEU:CD2   | 7:T:12:DT:C7     | 2.82                     | 0.56              |
| 5:M:156:ILE:HD13 | 5:M:156:ILE:N    | 2.20                     | 0.56              |
| 5:M:19:LEU:O     | 5:M:23:ILE:CG1   | 2.54                     | 0.56              |
| 2:C:873:ILE:N    | 2:C:873:ILE:HD13 | 2.20                     | 0.56              |
| 5:M:120:LEU:HD13 | 5:M:120:LEU:C    | 2.31                     | 0.56              |
| 5:M:127:GLN:NE2  | 5:M:186:ASP:N    | 2.54                     | 0.56              |
| 3:D:352:ARG:HE   | 3:D:465:GLN:HB3  | 1.71                     | 0.56              |
| 5:M:386:THR:HA   | 5:M:400:LYS:HG2  | 1.87                     | 0.56              |
| 5:M:127:GLN:NE2  | 5:M:186:ASP:HB2  | 2.21                     | 0.56              |
| 3:D:110:PRO:HG2  | 3:D:183:GLU:HB3  | 1.88                     | 0.56              |
| 1:A:33:ARG:NH1   | 1:A:199:ASP:OD2  | 2.39                     | 0.55              |
| 2:C:488:MET:SD   | 2:C:488:MET:N    | 2.75                     | 0.55              |
| 2:C:582:ASN:OD1  | 2:C:583:GLU:N    | 2.39                     | 0.55              |
| 2:C:955:GLN:HE21 | 2:C:955:GLN:CA   | 2.08                     | 0.55              |
| 3:D:126:LEU:O    | 3:D:220:ARG:NH1  | 2.40                     | 0.55              |
| 3:D:507:VAL:HG22 | 3:D:601:ILE:HD11 | 1.88                     | 0.55              |
| 5:M:279:ARG:C    | 5:M:279:ARG:HH21 | 2.13                     | 0.55              |
| 1:A:312:LEU:HD13 | 3:D:393:THR:HG23 | 1.88                     | 0.55              |
| 2:C:528:ARG:NH1  | 2:C:576:SER:O    | 2.39                     | 0.55              |
| 2:C:1275:VAL:HB  | 3:D:343:LEU:HG   | 1.88                     | 0.55              |
| 5:M:192:ALA:CB   | 5:M:198:CYS:HB2  | 2.35                     | 0.55              |
| 3:D:309:ASN:OD1  | 3:D:326:SER:OG   | 2.24                     | 0.55              |
| 5:M:398:GLU:HG2  | 5:M:401:TYR:H    | 1.71                     | 0.55              |
| 5:M:123:TYR:CE1  | 5:M:186:ASP:OD2  | 2.59                     | 0.55              |
| 1:A:18:GLN:NE2   | 1:A:20:SER:O     | 2.39                     | 0.55              |
| 2:C:1043:ALA:HB1 | 2:C:1044:PRO:HD2 | 1.78                     | 0.55              |
| 5:M:27:GLN:O     | 5:M:27:GLN:NE2   | 2.40                     | 0.55              |
| 5:M:287:VAL:HG11 | 5:M:342:ARG:HB3  | 1.87                     | 0.55              |
| 2:C:889:PRO:HA   | 2:C:913:VAL:HG12 | 1.88                     | 0.55              |
| 1:A:80:GLU:HG2   | 1:A:84:ASN:HD21  | 1.71                     | 0.55              |
| 1:A:131:CYS:SG   | 1:A:132:HIS:N    | 2.80                     | 0.55              |
| 3:D:480:ALA:HA   | 3:D:484:MET:HB2  | 1.89                     | 0.55              |
| 5:M:156:ILE:H    | 5:M:156:ILE:CD1  | 2.19                     | 0.55              |
| 1:B:106:GLY:HA3  | 1:B:136:GLU:HA   | 1.88                     | 0.55              |
| 5:M:340:LEU:HG   | 5:M:340:LEU:O    | 2.07                     | 0.55              |
| 5:M:392:SER:C    | 5:M:394:ARG:H    | 2.15                     | 0.55              |
| 2:C:873:ILE:HD13 | 2:C:873:ILE:O    | 2.06                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:M:390:LEU:CD1  | 5:M:399:LEU:HD22  | 2.36                     | 0.55              |
| 2:C:764:CYS:SG   | 2:C:831:ILE:HB    | 2.47                     | 0.54              |
| 2:C:873:ILE:H    | 2:C:873:ILE:CD1   | 2.20                     | 0.54              |
| 5:M:196:ARG:NH2  | 5:M:196:ARG:HG3   | 2.21                     | 0.54              |
| 2:C:185:ASP:OD2  | 2:C:200:ARG:NH2   | 2.41                     | 0.54              |
| 2:C:1013:GLN:HA  | 2:C:1013:GLN:OE1  | 2.07                     | 0.54              |
| 3:D:838:ARG:HE   | 3:D:1231:ARG:HH12 | 1.54                     | 0.54              |
| 5:M:123:TYR:CD1  | 5:M:123:TYR:C     | 2.85                     | 0.54              |
| 2:C:1107:MET:SD  | 2:C:1107:MET:N    | 2.81                     | 0.54              |
| 5:M:19:LEU:O     | 5:M:23:ILE:CD1    | 2.56                     | 0.54              |
| 5:M:26:LEU:H     | 5:M:26:LEU:CD1    | 2.17                     | 0.54              |
| 5:M:195:LEU:HD12 | 5:M:199:LEU:HD11  | 1.84                     | 0.54              |
| 2:C:902:LEU:HD23 | 2:C:910:ALA:HB2   | 1.87                     | 0.54              |
| 2:C:1018:TYR:CD1 | 2:C:1018:TYR:C    | 2.86                     | 0.54              |
| 3:D:77:ARG:NH1   | 5:M:146:ASP:O     | 2.40                     | 0.54              |
| 3:D:415:VAL:O    | 4:E:45:LYS:NZ     | 2.40                     | 0.54              |
| 5:M:184:ARG:CZ   | 5:M:201:ILE:HD13  | 2.35                     | 0.54              |
| 5:M:194:ASP:O    | 5:M:197:ASP:OD1   | 2.25                     | 0.54              |
| 2:C:488:MET:HE2  | 2:C:491:ASP:HA    | 1.89                     | 0.54              |
| 2:C:839:VAL:HA   | 2:C:1049:ILE:HG23 | 1.90                     | 0.54              |
| 3:D:510:LEU:HD11 | 3:D:624:ILE:HG23  | 1.90                     | 0.54              |
| 5:M:16:THR:CB    | 5:M:19:LEU:HB3    | 2.37                     | 0.54              |
| 1:A:256:PRO:HA   | 1:A:277:TYR:HB3   | 1.90                     | 0.54              |
| 5:M:271:TYR:CD1  | 5:M:271:TYR:N     | 2.74                     | 0.54              |
| 2:C:1211:ARG:NH2 | 2:C:1220:GLN:OE1  | 2.36                     | 0.54              |
| 2:C:841:ARG:O    | 2:C:841:ARG:HG3   | 2.08                     | 0.54              |
| 2:C:975:ILE:HG13 | 2:C:1014:LEU:HD12 | 1.90                     | 0.54              |
| 3:D:576:ARG:HD3  | 3:D:593:ASN:HA    | 1.89                     | 0.53              |
| 5:M:124:LEU:HD12 | 5:M:145:VAL:CG2   | 2.38                     | 0.53              |
| 2:C:1080:ASN:ND2 | 2:C:1085:MET:SD   | 2.81                     | 0.53              |
| 5:M:25:LEU:C     | 5:M:25:LEU:HD23   | 2.33                     | 0.53              |
| 7:T:12:DT:C5'    | 7:T:13:DG:H5'     | 2.25                     | 0.53              |
| 5:M:19:LEU:CD2   | 7:T:12:DT:H72     | 2.37                     | 0.53              |
| 5:M:354:PHE:CD1  | 5:M:359:GLU:HA    | 2.43                     | 0.53              |
| 5:M:377:HIS:HB2  | 7:T:13:DG:OP2     | 2.08                     | 0.53              |
| 3:D:644:MET:HG2  | 3:D:764:ARG:HD2   | 1.90                     | 0.53              |
| 5:M:22:ALA:HB2   | 5:M:328:TRP:HZ2   | 1.74                     | 0.53              |
| 1:B:64:VAL:HG12  | 1:B:66:HIS:H      | 1.74                     | 0.53              |
| 2:C:1022:LYS:HA  | 2:C:1022:LYS:HE2  | 1.89                     | 0.53              |
| 5:M:47:LEU:HD21  | 5:M:297:LEU:HD11  | 1.90                     | 0.53              |
| 5:M:259:ARG:HH11 | 5:M:259:ARG:CG    | 2.14                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:M:278:VAL:CG1  | 5:M:393:PRO:HD3  | 2.38                     | 0.53              |
| 7:T:29:DC:H2"    | 7:T:30:DC:C6     | 2.44                     | 0.53              |
| 5:M:421:ARG:CD   | 5:M:465:LEU:HD11 | 2.38                     | 0.53              |
| 2:C:850:ILE:HG22 | 2:C:886:LYS:HB2  | 1.91                     | 0.53              |
| 2:C:979:LEU:HD13 | 2:C:984:VAL:HB   | 1.90                     | 0.53              |
| 3:D:1024:THR:HA  | 3:D:1125:PRO:HB3 | 1.91                     | 0.53              |
| 5:M:28:LEU:HD13  | 5:M:28:LEU:O     | 2.08                     | 0.53              |
| 5:M:28:LEU:HD23  | 5:M:32:GLU:HB3   | 1.91                     | 0.53              |
| 5:M:133:PHE:HZ   | 5:M:181:ARG:HG3  | 1.74                     | 0.53              |
| 2:C:1032:LYS:HZ2 | 2:C:1032:LYS:CB  | 2.21                     | 0.53              |
| 5:M:431:GLU:CB   | 5:M:437:LEU:HG   | 2.39                     | 0.53              |
| 2:C:1027:LYS:HA  | 2:C:1030:GLU:HB3 | 1.92                     | 0.52              |
| 3:D:346:ARG:H    | 3:D:346:ARG:HD2  | 1.74                     | 0.52              |
| 3:D:1327:GLU:OE1 | 3:D:1329:THR:OG1 | 2.26                     | 0.52              |
| 4:E:44:ASP:OD1   | 4:E:45:LYS:N     | 2.42                     | 0.52              |
| 2:C:825:GLU:HB3  | 2:C:827:ARG:HG2  | 1.91                     | 0.52              |
| 3:D:833:GLU:OE1  | 3:D:1242:ARG:NH1 | 2.43                     | 0.52              |
| 1:B:183:ILE:HD13 | 1:B:205:MET:HE2  | 1.92                     | 0.52              |
| 2:C:840:SER:HB2  | 2:C:1048:LYS:H   | 1.74                     | 0.52              |
| 5:M:25:LEU:HD23  | 5:M:26:LEU:HD12  | 1.91                     | 0.52              |
| 5:M:259:ARG:HG3  | 5:M:259:ARG:NH1  | 2.21                     | 0.52              |
| 5:M:26:LEU:N     | 5:M:26:LEU:CD1   | 2.73                     | 0.52              |
| 5:M:127:GLN:NE2  | 5:M:186:ASP:H    | 2.07                     | 0.52              |
| 5:M:278:VAL:HG21 | 5:M:393:PRO:CG   | 2.39                     | 0.52              |
| 2:C:161:LYS:HA   | 2:C:170:VAL:HG12 | 1.92                     | 0.52              |
| 5:M:405:SER:HB2  | 7:T:21:DC:H4'    | 1.92                     | 0.52              |
| 2:C:150:HIS:HE1  | 2:C:536:GLY:HA3  | 1.74                     | 0.52              |
| 2:C:798:GLN:HB3  | 2:C:827:ARG:HH21 | 1.74                     | 0.52              |
| 2:C:148:GLN:HB2  | 2:C:511:LEU:HD21 | 1.92                     | 0.52              |
| 2:C:836:LEU:N    | 2:C:836:LEU:CD2  | 2.73                     | 0.52              |
| 2:C:902:LEU:HA   | 2:C:905:ILE:HD12 | 1.92                     | 0.52              |
| 2:C:935:THR:HG22 | 2:C:1048:LYS:HE2 | 1.92                     | 0.52              |
| 3:D:1268:ASN:OD1 | 3:D:1269:ALA:N   | 2.42                     | 0.52              |
| 5:M:400:LYS:HE3  | 6:N:-16:DT:OP1   | 2.10                     | 0.52              |
| 1:A:58:GLU:HG2   | 1:A:145:LYS:HE2  | 1.91                     | 0.52              |
| 1:A:182:ARG:HB3  | 1:A:206:GLU:HB3  | 1.91                     | 0.52              |
| 2:C:873:ILE:N    | 2:C:873:ILE:CD1  | 2.73                     | 0.52              |
| 2:C:1023:HIS:CE1 | 2:C:1027:LYS:HE3 | 2.45                     | 0.52              |
| 5:M:20:GLN:HA    | 5:M:23:ILE:HD11  | 1.91                     | 0.52              |
| 5:M:343:VAL:HG11 | 5:M:384:VAL:CG1  | 2.38                     | 0.52              |
| 5:M:399:LEU:CD2  | 5:M:399:LEU:N    | 2.73                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:N:-11:DC:N4    | 7:T:11:DG:H1     | 2.02                     | 0.52              |
| 2:C:797:GLY:HA3  | 2:C:1232:MET:O   | 2.10                     | 0.51              |
| 5:M:268:GLU:O    | 5:M:268:GLU:HG3  | 2.09                     | 0.51              |
| 5:M:287:VAL:CG2  | 5:M:345:ARG:HH11 | 2.22                     | 0.51              |
| 2:C:295:LYS:HE2  | 2:C:335:THR:HG21 | 1.91                     | 0.51              |
| 5:M:144:ILE:HD11 | 5:M:161:ILE:CB   | 2.37                     | 0.51              |
| 5:M:172:LEU:N    | 5:M:172:LEU:CD2  | 2.73                     | 0.51              |
| 5:M:278:VAL:HG11 | 5:M:393:PRO:HD3  | 1.91                     | 0.51              |
| 3:D:51:PRO:HB2   | 3:D:58:CYS:HA    | 1.92                     | 0.51              |
| 2:C:758:ARG:HD2  | 2:C:835:GLU:HB3  | 1.92                     | 0.51              |
| 5:M:277:LEU:CD1  | 5:M:288:GLU:HB3  | 2.41                     | 0.51              |
| 5:M:17:PRO:CA    | 6:N:-12:DA:C2    | 2.94                     | 0.51              |
| 2:C:836:LEU:HD23 | 2:C:836:LEU:C    | 2.35                     | 0.51              |
| 2:C:1022:LYS:NZ  | 2:C:1022:LYS:CB  | 2.73                     | 0.51              |
| 5:M:200:LEU:HD22 | 5:M:200:LEU:O    | 2.11                     | 0.51              |
| 5:M:431:GLU:HB2  | 5:M:437:LEU:HG   | 1.92                     | 0.51              |
| 2:C:697:LYS:O    | 2:C:799:ASN:ND2  | 2.43                     | 0.51              |
| 5:M:259:ARG:CG   | 5:M:259:ARG:NH1  | 2.73                     | 0.51              |
| 5:M:277:LEU:HD11 | 5:M:288:GLU:HB3  | 1.93                     | 0.51              |
| 2:C:592:ARG:NH1  | 2:C:654:ASP:O    | 2.43                     | 0.51              |
| 5:M:423:LEU:HA   | 5:M:426:LYS:HG2  | 1.93                     | 0.51              |
| 5:M:456:ARG:NH1  | 7:T:23:DT:H2"    | 2.23                     | 0.51              |
| 2:C:1219:GLU:OE1 | 3:D:634:ARG:NH1  | 2.44                     | 0.51              |
| 5:M:26:LEU:HG    | 5:M:336:ARG:CG   | 2.41                     | 0.51              |
| 5:M:49:GLU:CB    | 5:M:296:ARG:O    | 2.58                     | 0.51              |
| 5:M:377:HIS:CB   | 7:T:13:DG:OP2    | 2.59                     | 0.51              |
| 2:C:10:ARG:HH21  | 2:C:1181:PRO:HG2 | 1.76                     | 0.50              |
| 1:A:166:ARG:NH1  | 2:C:876:GLU:OE1  | 2.44                     | 0.50              |
| 1:B:97:GLU:HA    | 1:B:146:VAL:O    | 2.11                     | 0.50              |
| 2:C:1022:LYS:N   | 2:C:1022:LYS:HD2 | 2.26                     | 0.50              |
| 5:M:28:LEU:N     | 5:M:28:LEU:CD1   | 2.73                     | 0.50              |
| 5:M:409:THR:HG23 | 5:M:451:ILE:HA   | 1.92                     | 0.50              |
| 2:C:1291:LEU:O   | 2:C:1295:SER:OG  | 2.28                     | 0.50              |
| 3:D:291:ILE:HG23 | 5:M:303:TYR:CE1  | 2.47                     | 0.50              |
| 5:M:227:LEU:HD22 | 5:M:232:PHE:HE1  | 1.76                     | 0.50              |
| 5:M:390:LEU:C    | 5:M:390:LEU:CD2  | 2.85                     | 0.50              |
| 1:A:118:ASP:OD1  | 1:A:119:GLY:N    | 2.42                     | 0.50              |
| 2:C:1032:LYS:NZ  | 2:C:1032:LYS:CB  | 2.73                     | 0.50              |
| 3:D:982:LEU:HB2  | 3:D:995:TYR:HB2  | 1.92                     | 0.50              |
| 2:C:1017:GLN:HA  | 2:C:1017:GLN:OE1 | 2.12                     | 0.50              |
| 5:M:17:PRO:C     | 5:M:19:LEU:N     | 2.70                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:19:LEU:HD21   | 7:T:12:DT:C7      | 2.40                     | 0.50              |
| 5:M:247:LYS:O     | 5:M:250:VAL:HB    | 2.11                     | 0.50              |
| 2:C:877:VAL:O     | 2:C:877:VAL:HG13  | 2.12                     | 0.50              |
| 3:D:422:LEU:HD13  | 3:D:484:MET:HE1   | 1.93                     | 0.50              |
| 5:M:142:THR:O     | 5:M:146:ASP:HB3   | 2.12                     | 0.50              |
| 7:T:11:DG:OP2     | 7:T:11:DG:H8      | 1.94                     | 0.50              |
| 2:C:976:ARG:HA    | 2:C:979:LEU:HD23  | 1.92                     | 0.50              |
| 5:M:156:ILE:N     | 5:M:156:ILE:CD1   | 2.73                     | 0.50              |
| 5:M:279:ARG:CB    | 5:M:286:THR:HG22  | 2.42                     | 0.50              |
| 5:M:392:SER:C     | 5:M:394:ARG:N     | 2.70                     | 0.50              |
| 3:D:709:ARG:HG3   | 3:D:710:ASP:H     | 1.77                     | 0.50              |
| 3:D:437:PHE:HZ    | 3:D:453:VAL:HG21  | 1.77                     | 0.50              |
| 5:M:273:ILE:HG22  | 5:M:274:PRO:HD2   | 1.94                     | 0.50              |
| 2:C:704:MET:HB2   | 2:C:707:ALA:HB3   | 1.94                     | 0.49              |
| 5:M:340:LEU:HA    | 5:M:384:VAL:HG11  | 1.94                     | 0.49              |
| 2:C:805:MET:HE2   | 2:C:1225:VAL:HG21 | 1.94                     | 0.49              |
| 2:C:1209:GLN:HB3  | 2:C:1224:PRO:HB2  | 1.94                     | 0.49              |
| 3:D:842:ARG:HH21  | 3:D:1251:LYS:HG2  | 1.77                     | 0.49              |
| 5:M:456:ARG:NH1   | 7:T:24:DG:OP2     | 2.46                     | 0.49              |
| 2:C:723:VAL:O     | 2:C:735:LYS:N     | 2.41                     | 0.49              |
| 2:C:1032:LYS:HA   | 2:C:1032:LYS:HE3  | 1.93                     | 0.49              |
| 5:M:15:MET:HE3    | 6:N:-11:DC:C5'    | 2.41                     | 0.49              |
| 5:M:196:ARG:CD    | 5:M:196:ARG:C     | 2.86                     | 0.49              |
| 5:M:154:LEU:CD1   | 5:M:154:LEU:C     | 2.85                     | 0.49              |
| 2:C:995:ASP:OD1   | 2:C:995:ASP:N     | 2.46                     | 0.49              |
| 5:M:16:THR:CG2    | 5:M:20:GLN:N      | 2.69                     | 0.49              |
| 2:C:1037:THR:HG23 | 2:C:1037:THR:O    | 2.13                     | 0.49              |
| 5:M:386:THR:HG21  | 5:M:400:LYS:HZ1   | 1.78                     | 0.49              |
| 5:M:456:ARG:H     | 5:M:456:ARG:HE    | 1.61                     | 0.49              |
| 1:A:231:PHE:HZ    | 1:B:201:LEU:HD11  | 1.77                     | 0.49              |
| 2:C:836:LEU:CD2   | 2:C:836:LEU:C     | 2.86                     | 0.49              |
| 5:M:196:ARG:C     | 5:M:196:ARG:HD2   | 2.37                     | 0.49              |
| 5:M:349:GLU:C     | 5:M:351:GLN:N     | 2.68                     | 0.49              |
| 1:B:54:CYS:HB3    | 1:B:148:ARG:HD2   | 1.95                     | 0.49              |
| 2:C:677:ASN:N     | 2:C:677:ASN:OD1   | 2.45                     | 0.49              |
| 5:M:28:LEU:C      | 5:M:28:LEU:CD1    | 2.85                     | 0.49              |
| 5:M:387:GLN:N     | 5:M:387:GLN:NE2   | 2.60                     | 0.49              |
| 1:A:95:LYS:HE2    | 1:A:98:VAL:HG12   | 1.95                     | 0.49              |
| 2:C:942:ASP:HB3   | 2:C:946:LEU:HD13  | 1.93                     | 0.49              |
| 2:C:976:ARG:HA    | 2:C:979:LEU:CD2   | 2.43                     | 0.49              |
| 2:C:1315:MET:HB2  | 3:D:473:THR:HG21  | 1.95                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:290:ILE:HG12 | 3:D:293:ARG:HH22  | 1.77                     | 0.48              |
| 3:D:646:ILE:HD11 | 3:D:762:ASN:HD21  | 1.78                     | 0.48              |
| 5:M:23:ILE:CD1   | 5:M:23:ILE:C      | 2.86                     | 0.48              |
| 5:M:26:LEU:C     | 5:M:28:LEU:H      | 2.21                     | 0.48              |
| 5:M:184:ARG:HH11 | 5:M:205:GLN:NE2   | 2.08                     | 0.48              |
| 6:N:-10:DG:H1'   | 6:N:-9:DA:H5'     | 1.95                     | 0.48              |
| 1:A:68:TYR:HB3   | 2:C:929:ILE:HD11  | 1.93                     | 0.48              |
| 3:D:45:ASN:HD21  | 3:D:50:LYS:HG3    | 1.78                     | 0.48              |
| 5:M:405:SER:CB   | 7:T:21:DC:H4'     | 2.42                     | 0.48              |
| 2:C:269:ILE:HD11 | 2:C:274:ILE:HD11  | 1.95                     | 0.48              |
| 3:D:929:GLN:HB2  | 3:D:1138:LEU:HD13 | 1.95                     | 0.48              |
| 5:M:268:GLU:N    | 5:M:269:PRO:HD3   | 2.28                     | 0.48              |
| 5:M:295:PRO:O    | 5:M:297:LEU:HD22  | 2.13                     | 0.48              |
| 5:M:390:LEU:HB3  | 5:M:399:LEU:CD2   | 2.42                     | 0.48              |
| 5:M:391:HIS:CB   | 5:M:396:ILE:CG1   | 2.76                     | 0.48              |
| 5:M:399:LEU:HD23 | 5:M:399:LEU:N     | 2.28                     | 0.48              |
| 2:C:208:ILE:HD11 | 2:C:362:ALA:HB1   | 1.95                     | 0.48              |
| 2:C:833:ILE:HD13 | 2:C:1055:ALA:HB2  | 1.95                     | 0.48              |
| 3:D:460:ASP:OD1  | 3:D:460:ASP:N     | 2.46                     | 0.48              |
| 2:C:444:ASP:HB3  | 2:C:447:HIS:HB2   | 1.94                     | 0.48              |
| 2:C:1065:LYS:HG2 | 2:C:1235:LEU:HD12 | 1.95                     | 0.48              |
| 5:M:276:VAL:O    | 5:M:276:VAL:HG12  | 2.14                     | 0.48              |
| 2:C:672:GLU:HB2  | 3:D:767:LEU:HB2   | 1.96                     | 0.48              |
| 5:M:133:PHE:CZ   | 5:M:181:ARG:HG3   | 2.47                     | 0.48              |
| 2:C:870:ILE:HG22 | 2:C:870:ILE:O     | 2.13                     | 0.48              |
| 3:D:923:ILE:O    | 3:D:1241:TYR:OH   | 2.31                     | 0.48              |
| 2:C:918:LEU:C    | 2:C:918:LEU:CD1   | 2.86                     | 0.48              |
| 2:C:1108:ASN:O   | 2:C:1111:GLN:HG2  | 2.14                     | 0.48              |
| 5:M:279:ARG:CZ   | 5:M:281:VAL:HB    | 2.44                     | 0.48              |
| 2:C:844:LYS:O    | 2:C:844:LYS:HG2   | 2.07                     | 0.48              |
| 3:D:120:LEU:HB2  | 3:D:121:PRO:HD3   | 1.95                     | 0.48              |
| 3:D:394:ILE:HG21 | 5:M:130:LEU:HD12  | 1.95                     | 0.48              |
| 6:N:-9:DA:C1'    | 6:N:-8:DT:H5'     | 2.32                     | 0.48              |
| 2:C:425:ILE:HG22 | 2:C:429:MET:HE2   | 1.96                     | 0.47              |
| 2:C:633:LEU:HA   | 2:C:645:PHE:O     | 2.13                     | 0.47              |
| 2:C:960:LEU:C    | 2:C:960:LEU:CD1   | 2.85                     | 0.47              |
| 5:M:176:GLU:O    | 5:M:180:LYS:HB2   | 2.13                     | 0.47              |
| 5:M:297:LEU:HB3  | 5:M:330:ILE:HD12  | 1.92                     | 0.47              |
| 5:M:390:LEU:HD13 | 5:M:397:PHE:O     | 2.14                     | 0.47              |
| 2:C:549:ASP:OD1  | 2:C:550:VAL:N     | 2.45                     | 0.47              |
| 2:C:841:ARG:HH22 | 2:C:1046:VAL:HG22 | 1.79                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:M:387:GLN:NE2   | 5:M:387:GLN:H     | 2.11                     | 0.47              |
| 3:D:371:LYS:HD2   | 3:D:445:LYS:HE3   | 1.97                     | 0.47              |
| 5:M:390:LEU:HD13  | 5:M:399:LEU:HD22  | 1.95                     | 0.47              |
| 2:C:810:TYR:O     | 2:C:815:SER:OG    | 2.23                     | 0.47              |
| 3:D:515:ARG:NH1   | 3:D:718:SER:O     | 2.46                     | 0.47              |
| 3:D:980:THR:OG1   | 3:D:997:VAL:O     | 2.33                     | 0.47              |
| 5:M:227:LEU:C     | 5:M:227:LEU:CD1   | 2.86                     | 0.47              |
| 5:M:377:HIS:ND1   | 5:M:379:SER:OG    | 2.47                     | 0.47              |
| 5:M:399:LEU:HD23  | 5:M:399:LEU:H     | 1.79                     | 0.47              |
| 2:C:835:GLU:HG3   | 2:C:1053:TYR:CE1  | 2.50                     | 0.47              |
| 5:M:26:LEU:CB     | 5:M:336:ARG:HD2   | 2.23                     | 0.47              |
| 1:B:30:PRO:HB3    | 1:B:190:ALA:HB3   | 1.96                     | 0.47              |
| 2:C:844:LYS:CE    | 5:M:271:TYR:HB3   | 2.44                     | 0.47              |
| 2:C:852:ALA:HB2   | 2:C:869:GLY:N     | 2.30                     | 0.47              |
| 2:C:971:LEU:HD12  | 2:C:971:LEU:HA    | 1.72                     | 0.47              |
| 2:C:1043:ALA:HB3  | 2:C:1046:VAL:CG2  | 2.45                     | 0.47              |
| 3:D:1034:PHE:N    | 3:D:1081:VAL:O    | 2.48                     | 0.47              |
| 1:A:166:ARG:HH22  | 2:C:876:GLU:CD    | 2.21                     | 0.47              |
| 2:C:197:ARG:HH21  | 2:C:203:LYS:HG2   | 1.79                     | 0.47              |
| 2:C:1030:GLU:OE1  | 2:C:1030:GLU:HA   | 2.15                     | 0.47              |
| 2:C:1185:PRO:HD2  | 2:C:1189:GLY:HA2  | 1.96                     | 0.47              |
| 5:M:196:ARG:HH21  | 5:M:196:ARG:CB    | 2.27                     | 0.47              |
| 5:M:278:VAL:CG1   | 5:M:392:SER:HB3   | 2.45                     | 0.47              |
| 2:C:845:LEU:HD11  | 5:M:271:TYR:CE2   | 2.50                     | 0.47              |
| 2:C:848:GLU:N     | 2:C:848:GLU:CD    | 2.72                     | 0.47              |
| 5:M:26:LEU:C      | 5:M:26:LEU:HD22   | 2.40                     | 0.47              |
| 5:M:390:LEU:HD11  | 5:M:402:PHE:CZ    | 2.50                     | 0.47              |
| 7:T:0:DC:H2''     | 7:T:1:DA:C8       | 2.50                     | 0.47              |
| 1:A:32:GLU:OE2    | 1:B:150:ARG:NH2   | 2.37                     | 0.46              |
| 1:A:44:ARG:HG3    | 1:A:183:ILE:HG22  | 1.96                     | 0.46              |
| 1:A:66:HIS:HD2    | 1:A:68:TYR:HB2    | 1.80                     | 0.46              |
| 1:A:158:ARG:NH2   | 1:A:173:VAL:O     | 2.45                     | 0.46              |
| 2:C:1291:LEU:HD11 | 3:D:1351:VAL:HG13 | 1.97                     | 0.46              |
| 5:M:406:HIS:O     | 7:T:22:DG:C5'     | 2.63                     | 0.46              |
| 5:M:421:ARG:HD3   | 5:M:465:LEU:HD21  | 1.97                     | 0.46              |
| 1:B:33:ARG:O      | 1:B:33:ARG:NH1    | 2.47                     | 0.46              |
| 5:M:180:LYS:O     | 5:M:180:LYS:NZ    | 2.43                     | 0.46              |
| 5:M:436:PRO:HB2   | 5:M:470:SER:HB3   | 1.97                     | 0.46              |
| 2:C:715:THR:HG22  | 2:C:786:GLY:H     | 1.79                     | 0.46              |
| 3:D:591:ILE:HG23  | 3:D:592:VAL:HG13  | 1.98                     | 0.46              |
| 5:M:264:ILE:HG23  | 5:M:264:ILE:O     | 2.14                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1125:GLY:HA3  | 2:C:1179:GLY:HA2  | 1.98                     | 0.46              |
| 3:D:250:ARG:HB3   | 3:D:265:LEU:HD23  | 1.97                     | 0.46              |
| 3:D:308:ASP:OD2   | 3:D:311:ARG:NH1   | 2.49                     | 0.46              |
| 3:D:679:TYR:OH    | 3:D:754:ILE:O     | 2.29                     | 0.46              |
| 3:D:846:GLU:HA    | 3:D:860:ARG:HA    | 1.96                     | 0.46              |
| 3:D:1328:THR:O    | 3:D:1329:THR:C    | 2.59                     | 0.46              |
| 5:M:20:GLN:C      | 5:M:20:GLN:NE2    | 2.73                     | 0.46              |
| 2:C:143:ARG:NH2   | 2:C:512:SER:O     | 2.43                     | 0.46              |
| 2:C:187:GLU:HB2   | 2:C:195:PHE:HB2   | 1.98                     | 0.46              |
| 2:C:1251:TYR:HB3  | 2:C:1257:GLN:C    | 2.41                     | 0.46              |
| 3:D:60:ARG:H      | 3:D:90:VAL:HG22   | 1.80                     | 0.46              |
| 5:M:142:THR:HA    | 5:M:145:VAL:HG12  | 1.98                     | 0.46              |
| 1:B:174:ASP:OD1   | 1:B:174:ASP:N     | 2.49                     | 0.46              |
| 2:C:538:LEU:HD13  | 2:C:538:LEU:H     | 1.81                     | 0.46              |
| 2:C:732:ILE:HD11  | 2:C:769:PRO:HB3   | 1.97                     | 0.46              |
| 2:C:746:ALA:HB2   | 2:C:967:LEU:HD21  | 1.97                     | 0.46              |
| 2:C:1254:VAL:HG12 | 2:C:1255:THR:HG23 | 1.97                     | 0.46              |
| 5:M:173:GLU:N     | 5:M:173:GLU:CD    | 2.73                     | 0.46              |
| 5:M:386:THR:HA    | 5:M:400:LYS:CG    | 2.45                     | 0.46              |
| 7:T:20:DT:H2''    | 7:T:21:DC:C6      | 2.51                     | 0.46              |
| 2:C:414:ILE:HD13  | 2:C:414:ILE:H     | 1.81                     | 0.46              |
| 5:M:21:GLN:C      | 5:M:23:ILE:N      | 2.70                     | 0.46              |
| 5:M:27:GLN:NE2    | 5:M:27:GLN:C      | 2.73                     | 0.46              |
| 1:A:312:LEU:CD2   | 5:M:181:ARG:NH1   | 2.75                     | 0.46              |
| 1:B:197:ASP:OD1   | 1:B:197:ASP:N     | 2.49                     | 0.46              |
| 2:C:921:PRO:HB2   | 2:C:924:VAL:CG2   | 2.46                     | 0.46              |
| 2:C:1104:PRO:HG3  | 3:D:725:MET:HE2   | 1.97                     | 0.46              |
| 2:C:854:ILE:H     | 2:C:854:ILE:CD1   | 1.96                     | 0.45              |
| 2:C:1296:ASP:OD2  | 3:D:345:LYS:NZ    | 2.38                     | 0.45              |
| 5:M:46:LEU:HD11   | 5:M:322:ASN:HB3   | 1.98                     | 0.45              |
| 2:C:179:TYR:OH    | 2:C:462:ASN:OD1   | 2.28                     | 0.45              |
| 2:C:1048:LYS:HE2  | 2:C:1048:LYS:HB2  | 1.78                     | 0.45              |
| 7:T:6:DT:H2''     | 7:T:7:DG:C8       | 2.51                     | 0.45              |
| 2:C:1023:HIS:HD1  | 2:C:1023:HIS:C    | 2.23                     | 0.45              |
| 3:D:352:ARG:NE    | 3:D:465:GLN:HB3   | 2.31                     | 0.45              |
| 7:T:8:DA:H1'      | 7:T:9:DT:H5'      | 1.97                     | 0.45              |
| 3:D:1227:HIS:O    | 3:D:1230:THR:OG1  | 2.32                     | 0.45              |
| 5:M:341:LEU:HD23  | 5:M:342:ARG:HG2   | 1.99                     | 0.45              |
| 1:A:180:VAL:O     | 1:A:207:THR:HA    | 2.16                     | 0.45              |
| 2:C:806:PRO:HA    | 2:C:811:ASN:HD21  | 1.81                     | 0.45              |
| 2:C:1042:LEU:HD12 | 2:C:1042:LEU:N    | 2.22                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1253:LEU:HD12 | 5:M:114:GLY:HA3   | 1.98                     | 0.45              |
| 3:D:70:CYS:CB     | 3:D:72:CYS:SG     | 3.05                     | 0.45              |
| 5:M:184:ARG:NH1   | 5:M:205:GLN:HE22  | 2.10                     | 0.45              |
| 1:A:155:ALA:O     | 1:A:159:ILE:HG12  | 2.17                     | 0.45              |
| 2:C:206:ALA:O     | 2:C:208:ILE:N     | 2.46                     | 0.45              |
| 3:D:814:CYS:CB    | 3:D:895:CYS:SG    | 3.05                     | 0.45              |
| 3:D:1155:ILE:HG21 | 3:D:1190:ILE:HG12 | 1.98                     | 0.45              |
| 5:M:144:ILE:HD11  | 5:M:161:ILE:CG1   | 2.46                     | 0.45              |
| 5:M:350:GLN:OE1   | 5:M:370:ILE:HD13  | 2.17                     | 0.45              |
| 1:B:232:VAL:HG13  | 1:B:234:LEU:H     | 1.82                     | 0.45              |
| 5:M:299:ILE:HD12  | 5:M:300:ASN:H     | 1.81                     | 0.45              |
| 2:C:1269:ARG:HA   | 3:D:346:ARG:HA    | 1.98                     | 0.45              |
| 5:M:345:ARG:HD3   | 5:M:346:CYS:SG    | 2.57                     | 0.45              |
| 5:M:349:GLU:O     | 5:M:352:GLN:CG    | 2.58                     | 0.45              |
| 2:C:27:LEU:O      | 2:C:528:ARG:NH2   | 2.50                     | 0.45              |
| 2:C:496:LYS:HB2   | 2:C:497:PRO:HD3   | 1.99                     | 0.45              |
| 2:C:932:GLN:NE2   | 2:C:932:GLN:CA    | 2.73                     | 0.45              |
| 5:M:349:GLU:C     | 5:M:351:GLN:H     | 2.25                     | 0.45              |
| 6:N:-33:DG:H2''   | 6:N:-32:DA:N7     | 2.31                     | 0.45              |
| 1:B:91:ARG:HB3    | 1:B:122:GLU:HB2   | 1.99                     | 0.45              |
| 2:C:805:MET:O     | 2:C:811:ASN:ND2   | 2.50                     | 0.45              |
| 3:D:453:VAL:O     | 3:D:456:ALA:HB3   | 2.17                     | 0.45              |
| 3:D:842:ARG:HG3   | 3:D:882:VAL:HG21  | 1.99                     | 0.45              |
| 5:M:180:LYS:HA    | 5:M:180:LYS:HD2   | 1.61                     | 0.45              |
| 2:C:854:ILE:HD12  | 2:C:854:ILE:N     | 2.07                     | 0.44              |
| 3:D:1181:ASP:HA   | 3:D:1185:PRO:HB3  | 1.99                     | 0.44              |
| 5:M:123:TYR:CD1   | 5:M:123:TYR:O     | 2.70                     | 0.44              |
| 2:C:661:VAL:HG21  | 2:C:1186:VAL:HG11 | 1.99                     | 0.44              |
| 3:D:65:VAL:HG13   | 3:D:66:LYS:HG2    | 1.99                     | 0.44              |
| 5:M:25:LEU:HD23   | 5:M:26:LEU:N      | 2.33                     | 0.44              |
| 5:M:385:THR:O     | 5:M:399:LEU:HB2   | 2.17                     | 0.44              |
| 2:C:877:VAL:HG21  | 2:C:883:LEU:HD13  | 2.00                     | 0.44              |
| 2:C:964:LEU:C     | 2:C:964:LEU:CD1   | 2.90                     | 0.44              |
| 3:D:600:ALA:HA    | 3:D:603:LYS:HE3   | 1.99                     | 0.44              |
| 5:M:33:LEU:O      | 5:M:33:LEU:HD23   | 2.17                     | 0.44              |
| 5:M:454:ALA:HB1   | 5:M:456:ARG:NE    | 2.32                     | 0.44              |
| 3:D:381:ILE:HD11  | 3:D:412:LEU:HD13  | 1.99                     | 0.44              |
| 3:D:640:GLY:N     | 3:D:643:ASP:OD2   | 2.43                     | 0.44              |
| 5:M:24:ARG:NH1    | 5:M:25:LEU:HA     | 2.33                     | 0.44              |
| 5:M:390:LEU:HD12  | 5:M:399:LEU:HD22  | 1.99                     | 0.44              |
| 2:C:310:ILE:H     | 2:C:310:ILE:HG13  | 1.59                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:824:PRO:HB3  | 3:D:834:PRO:HA    | 1.99                     | 0.44              |
| 3:D:919:ALA:C    | 3:D:921:GLN:H     | 2.25                     | 0.44              |
| 2:C:637:ARG:HG2  | 2:C:642:SER:HB3   | 2.00                     | 0.44              |
| 2:C:1038:GLN:O   | 2:C:1038:GLN:HG3  | 2.13                     | 0.44              |
| 3:D:478:LEU:HB2  | 4:E:20:VAL:HG13   | 1.99                     | 0.44              |
| 5:M:147:ALA:HB1  | 5:M:156:ILE:HD12  | 1.99                     | 0.44              |
| 5:M:202:GLN:O    | 5:M:206:PHE:CD1   | 2.71                     | 0.44              |
| 2:C:1088:ASP:HA  | 2:C:1213:TYR:HD1  | 1.83                     | 0.44              |
| 5:M:391:HIS:ND1  | 5:M:391:HIS:C     | 2.73                     | 0.44              |
| 2:C:519:ASN:OD1  | 2:C:522:SER:N     | 2.51                     | 0.44              |
| 3:D:95:THR:HG23  | 3:D:98:ARG:HH22   | 1.83                     | 0.44              |
| 3:D:430:HIS:CE1  | 3:D:432:LEU:HB2   | 2.52                     | 0.44              |
| 5:M:17:PRO:HG3   | 6:N:-12:DA:C5     | 2.52                     | 0.44              |
| 6:N:-13:DC:N3    | 7:T:13:DG:N2      | 2.50                     | 0.44              |
| 2:C:738:GLU:HA   | 2:C:741:MET:HE2   | 1.99                     | 0.44              |
| 2:C:964:LEU:HD22 | 2:C:1025:PHE:CB   | 2.48                     | 0.43              |
| 2:C:1050:VAL:O   | 2:C:1050:VAL:HG13 | 2.18                     | 0.43              |
| 3:D:378:LYS:HB3  | 3:D:379:PRO:HD3   | 1.99                     | 0.43              |
| 3:D:466:MET:HG3  | 3:D:467:ALA:H     | 1.83                     | 0.43              |
| 4:E:66:VAL:HG22  | 4:E:69:ARG:HH12   | 1.83                     | 0.43              |
| 5:M:140:ILE:CG1  | 5:M:165:ILE:HD13  | 2.44                     | 0.43              |
| 1:A:180:VAL:HG23 | 1:A:181:GLU:H     | 1.83                     | 0.43              |
| 1:A:228:LEU:HD13 | 1:B:224:LEU:HB3   | 2.00                     | 0.43              |
| 2:C:559:CYS:N    | 2:C:574:SER:O     | 2.51                     | 0.43              |
| 2:C:921:PRO:HB2  | 2:C:924:VAL:HG23  | 2.00                     | 0.43              |
| 3:D:267:ASP:HA   | 3:D:270:ARG:HG2   | 1.99                     | 0.43              |
| 2:C:159:SER:HB2  | 2:C:442:VAL:HG11  | 2.00                     | 0.43              |
| 2:C:1073:LYS:H   | 2:C:1073:LYS:HD3  | 1.84                     | 0.43              |
| 5:M:123:TYR:C    | 5:M:123:TYR:HD1   | 2.26                     | 0.43              |
| 5:M:223:HIS:HB3  | 5:M:235:LEU:HD21  | 2.00                     | 0.43              |
| 5:M:329:LEU:HD13 | 5:M:329:LEU:O     | 2.18                     | 0.43              |
| 5:M:406:HIS:HE1  | 7:T:22:DG:H4'     | 1.81                     | 0.43              |
| 1:B:48:LEU:HD11  | 3:D:534:GLU:HG3   | 2.00                     | 0.43              |
| 2:C:1047:LEU:O   | 2:C:1047:LEU:HD12 | 2.18                     | 0.43              |
| 5:M:26:LEU:CG    | 5:M:336:ARG:CG    | 2.97                     | 0.43              |
| 7:T:32:DT:H2''   | 7:T:33:DC:C6      | 2.54                     | 0.43              |
| 1:B:55:ALA:HB3   | 1:B:175:ALA:HB1   | 2.00                     | 0.43              |
| 2:C:801:ARG:HB2  | 2:C:1229:TYR:CE2  | 2.54                     | 0.43              |
| 3:D:72:CYS:SG    | 3:D:88:CYS:CB     | 3.07                     | 0.43              |
| 5:M:19:LEU:CD2   | 7:T:12:DT:H71     | 2.48                     | 0.43              |
| 2:C:966:ILE:HA   | 2:C:966:ILE:HD12  | 1.72                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:979:LEU:HD13  | 2:C:984:VAL:CB    | 2.48                     | 0.43              |
| 5:M:22:ALA:HB2    | 5:M:328:TRP:CZ2   | 2.53                     | 0.43              |
| 3:D:39:LYS:O      | 3:D:277:ASN:ND2   | 2.31                     | 0.43              |
| 3:D:843:VAL:HG22  | 3:D:863:LEU:HD13  | 2.00                     | 0.43              |
| 5:M:19:LEU:HA     | 5:M:22:ALA:HB3    | 1.99                     | 0.43              |
| 1:A:60:GLU:HB3    | 1:A:170:ARG:HG3   | 1.99                     | 0.43              |
| 2:C:347:ILE:HD11  | 2:C:433:ILE:HD13  | 2.00                     | 0.43              |
| 1:B:144:ILE:HD13  | 1:B:144:ILE:H     | 1.84                     | 0.43              |
| 2:C:474:ALA:HA    | 2:C:477:GLU:HG2   | 2.00                     | 0.43              |
| 2:C:877:VAL:HG21  | 2:C:883:LEU:CD1   | 2.48                     | 0.43              |
| 2:C:1268:GLN:HG2  | 3:D:350:SER:HB2   | 2.00                     | 0.43              |
| 5:M:21:GLN:NE2    | 5:M:328:TRP:CZ2   | 2.87                     | 0.43              |
| 5:M:131:THR:HB    | 5:M:132:PRO:HD2   | 2.01                     | 0.43              |
| 1:A:195:ARG:HG2   | 1:A:196:THR:H     | 1.84                     | 0.42              |
| 1:A:221:ALA:HB1   | 1:B:228:LEU:HD23  | 2.00                     | 0.42              |
| 2:C:1004:ASP:HA   | 2:C:1008:GLN:NE2  | 2.33                     | 0.42              |
| 5:M:193:LYS:C     | 5:M:193:LYS:CD    | 2.90                     | 0.42              |
| 5:M:277:LEU:HD11  | 5:M:289:LEU:CD2   | 2.49                     | 0.42              |
| 5:M:456:ARG:HG2   | 5:M:457:THR:N     | 2.33                     | 0.42              |
| 2:C:758:ARG:CD    | 2:C:1053:TYR:CE2  | 3.02                     | 0.42              |
| 2:C:841:ARG:NH2   | 2:C:1046:VAL:HG22 | 2.34                     | 0.42              |
| 3:D:29:MET:HE3    | 3:D:29:MET:HB3    | 1.97                     | 0.42              |
| 3:D:102:MET:HE2   | 3:D:243:PRO:HB2   | 2.00                     | 0.42              |
| 5:M:280:LYS:O     | 5:M:280:LYS:HG2   | 2.18                     | 0.42              |
| 7:T:7:DG:H4'      | 7:T:8:DA:OP1      | 2.19                     | 0.42              |
| 1:A:51:MET:SD     | 1:A:52:PRO:HD2    | 2.59                     | 0.42              |
| 1:A:98:VAL:O      | 1:A:145:LYS:HA    | 2.19                     | 0.42              |
| 2:C:1182:ILE:HG22 | 2:C:1183:ALA:H    | 1.84                     | 0.42              |
| 5:M:36:GLU:HA     | 5:M:39:GLN:HB3    | 2.01                     | 0.42              |
| 5:M:144:ILE:CD1   | 5:M:161:ILE:CD1   | 2.68                     | 0.42              |
| 5:M:386:THR:O     | 5:M:388:LYS:NZ    | 2.53                     | 0.42              |
| 2:C:954:LYS:C     | 2:C:954:LYS:CD    | 2.90                     | 0.42              |
| 3:D:801:VAL:O     | 3:D:805:GLN:HB2   | 2.19                     | 0.42              |
| 5:M:456:ARG:HD2   | 7:T:23:DT:H2''    | 1.99                     | 0.42              |
| 1:A:80:GLU:HG2    | 1:A:84:ASN:ND2    | 2.33                     | 0.42              |
| 5:M:33:LEU:C      | 5:M:33:LEU:CD2    | 2.91                     | 0.42              |
| 5:M:140:ILE:HG12  | 5:M:165:ILE:HD11  | 1.99                     | 0.42              |
| 5:M:180:LYS:HD2   | 5:M:183:GLN:HG3   | 2.00                     | 0.42              |
| 6:N:-10:DG:C2     | 6:N:-9:DA:C4      | 3.07                     | 0.42              |
| 2:C:619:ALA:HB2   | 2:C:654:ASP:HB2   | 2.02                     | 0.42              |
| 3:D:746:LEU:HD23  | 3:D:758:PRO:HB3   | 2.00                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:1237:VAL:O   | 3:D:1240:VAL:HG12 | 2.19                     | 0.42              |
| 5:M:362:MET:SD   | 5:M:418:THR:OG1   | 2.75                     | 0.42              |
| 1:A:35:PHE:HA    | 1:A:38:THR:HG22   | 2.00                     | 0.42              |
| 2:C:678:ARG:HA   | 2:C:681:MET:HG2   | 2.01                     | 0.42              |
| 2:C:865:LEU:N    | 2:C:865:LEU:CD2   | 2.82                     | 0.42              |
| 2:C:992:LEU:HA   | 2:C:993:PRO:HD2   | 1.91                     | 0.42              |
| 2:C:1099:ASN:OD1 | 2:C:1101:LEU:HB2  | 2.19                     | 0.42              |
| 2:C:1278:LEU:HB3 | 2:C:1283:ALA:HB3  | 2.02                     | 0.42              |
| 5:M:277:LEU:HD11 | 5:M:289:LEU:HD22  | 2.01                     | 0.42              |
| 3:D:69:GLU:HB3   | 3:D:76:LYS:HA     | 2.01                     | 0.42              |
| 3:D:1146:GLU:OE1 | 3:D:1309:ILE:N    | 2.53                     | 0.42              |
| 3:D:1257:VAL:HA  | 3:D:1260:MET:HE2  | 2.01                     | 0.42              |
| 5:M:15:MET:HE3   | 6:N:-11:DC:O4'    | 2.20                     | 0.42              |
| 2:C:704:MET:HE3  | 2:C:707:ALA:HB3   | 2.02                     | 0.42              |
| 5:M:210:THR:HA   | 5:M:211:PRO:HD3   | 1.90                     | 0.42              |
| 5:M:338:ASP:OD1  | 5:M:342:ARG:NE    | 2.53                     | 0.42              |
| 5:M:354:PHE:HD1  | 5:M:359:GLU:HA    | 1.84                     | 0.42              |
| 2:C:972:PHE:CE1  | 2:C:993:PRO:HB3   | 2.55                     | 0.42              |
| 5:M:19:LEU:CD2   | 5:M:23:ILE:HG13   | 2.49                     | 0.42              |
| 5:M:179:LEU:HD13 | 5:M:179:LEU:C     | 2.44                     | 0.42              |
| 5:M:425:LYS:HD2  | 5:M:465:LEU:HD13  | 2.02                     | 0.42              |
| 2:C:559:CYS:HB3  | 2:C:574:SER:HB3   | 2.02                     | 0.41              |
| 2:C:1272:GLU:HA  | 2:C:1275:VAL:HG12 | 2.02                     | 0.41              |
| 3:D:364:HIS:HB3  | 3:D:487:THR:HG23  | 2.02                     | 0.41              |
| 5:M:19:LEU:CD1   | 5:M:19:LEU:C      | 2.86                     | 0.41              |
| 5:M:124:LEU:CD1  | 5:M:145:VAL:CG2   | 2.98                     | 0.41              |
| 2:C:217:THR:HG23 | 2:C:351:LEU:HD11  | 2.02                     | 0.41              |
| 3:D:491:LEU:HB2  | 3:D:904:ALA:HA    | 2.01                     | 0.41              |
| 5:M:387:GLN:N    | 5:M:387:GLN:CD    | 2.79                     | 0.41              |
| 1:A:111:THR:HA   | 1:A:129:VAL:HA    | 2.02                     | 0.41              |
| 2:C:189:ASP:HB2  | 2:C:195:PHE:CE2   | 2.55                     | 0.41              |
| 2:C:701:GLY:HA3  | 2:C:1182:ILE:O    | 2.21                     | 0.41              |
| 2:C:1017:GLN:N   | 2:C:1017:GLN:CD   | 2.78                     | 0.41              |
| 2:C:1035:LYS:HE3 | 2:C:1035:LYS:HB2  | 1.22                     | 0.41              |
| 3:D:1178:THR:HB  | 3:D:1179:PRO:HD3  | 2.02                     | 0.41              |
| 2:C:67:GLU:HB2   | 2:C:103:VAL:HB    | 2.02                     | 0.41              |
| 2:C:758:ARG:HD3  | 2:C:1053:TYR:CE2  | 2.56                     | 0.41              |
| 5:M:145:VAL:C    | 5:M:148:VAL:HG23  | 2.45                     | 0.41              |
| 5:M:162:VAL:HG21 | 5:M:172:LEU:CD2   | 2.33                     | 0.41              |
| 2:C:862:LEU:HD12 | 2:C:862:LEU:HA    | 1.82                     | 0.41              |
| 2:C:979:LEU:C    | 2:C:979:LEU:CD1   | 2.86                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:M:456:ARG:CG   | 7:T:23:DT:C6      | 3.02                     | 0.41              |
| 1:A:29:GLU:HB3   | 1:A:30:PRO:HD3    | 2.03                     | 0.41              |
| 1:A:38:THR:HB    | 1:B:45:ARG:HG2    | 2.02                     | 0.41              |
| 5:M:250:VAL:O    | 5:M:254:GLN:N     | 2.50                     | 0.41              |
| 1:B:59:VAL:HG12  | 1:B:144:ILE:HG22  | 2.03                     | 0.41              |
| 1:B:113:ALA:HB2  | 1:B:126:PRO:HB2   | 2.02                     | 0.41              |
| 2:C:69:GLN:HB2   | 2:C:101:ARG:HB3   | 2.03                     | 0.41              |
| 2:C:421:SER:OG   | 2:C:423:ASP:OD1   | 2.33                     | 0.41              |
| 2:C:887:VAL:HB   | 2:C:913:VAL:HB    | 2.02                     | 0.41              |
| 5:M:123:TYR:CE1  | 5:M:186:ASP:HB2   | 2.56                     | 0.41              |
| 5:M:294:ILE:HD12 | 5:M:295:PRO:N     | 2.36                     | 0.41              |
| 5:M:391:HIS:O    | 5:M:391:HIS:CG    | 2.70                     | 0.41              |
| 2:C:592:ARG:NH2  | 2:C:655:VAL:O     | 2.51                     | 0.41              |
| 2:C:936:ARG:O    | 2:C:936:ARG:HG2   | 2.20                     | 0.41              |
| 5:M:283:GLY:O    | 5:M:284:ARG:HG3   | 2.20                     | 0.41              |
| 5:M:294:ILE:HA   | 5:M:295:PRO:HD3   | 1.90                     | 0.41              |
| 5:M:420:ILE:O    | 5:M:424:VAL:HG23  | 2.20                     | 0.41              |
| 1:A:68:TYR:HB2   | 2:C:929:ILE:HD13  | 1.99                     | 0.41              |
| 2:C:366:ILE:H    | 2:C:366:ILE:HG13  | 1.65                     | 0.41              |
| 2:C:490:GLN:HE21 | 2:C:490:GLN:HB2   | 1.65                     | 0.41              |
| 2:C:696:ASP:OD2  | 2:C:799:ASN:ND2   | 2.33                     | 0.41              |
| 2:C:838:CYS:O    | 2:C:838:CYS:SG    | 2.79                     | 0.41              |
| 2:C:1030:GLU:C   | 2:C:1030:GLU:CD   | 2.86                     | 0.41              |
| 3:D:422:LEU:HG   | 3:D:469:HIS:HB2   | 2.02                     | 0.41              |
| 3:D:1330:ARG:O   | 3:D:1333:THR:OG1  | 2.36                     | 0.41              |
| 5:M:17:PRO:HG3   | 6:N:-12:DA:N3     | 2.34                     | 0.41              |
| 5:M:28:LEU:HD23  | 5:M:32:GLU:HG2    | 2.02                     | 0.41              |
| 5:M:124:LEU:CD1  | 5:M:124:LEU:C     | 2.94                     | 0.41              |
| 5:M:215:GLU:H    | 5:M:215:GLU:HG2   | 1.63                     | 0.41              |
| 5:M:390:LEU:C    | 5:M:390:LEU:HD23  | 2.46                     | 0.41              |
| 7:T:7:DG:H1'     | 7:T:8:DA:H5''     | 2.02                     | 0.41              |
| 2:C:886:LYS:HZ3  | 2:C:886:LYS:HG2   | 1.68                     | 0.41              |
| 2:C:1022:LYS:CA  | 2:C:1022:LYS:NZ   | 2.73                     | 0.41              |
| 3:D:502:PRO:HG2  | 3:D:601:ILE:HD12  | 2.03                     | 0.41              |
| 5:M:24:ARG:O     | 5:M:27:GLN:HG3    | 2.21                     | 0.41              |
| 5:M:196:ARG:HH21 | 5:M:196:ARG:HG3   | 1.79                     | 0.41              |
| 1:A:312:LEU:CA   | 5:M:181:ARG:HH11  | 2.34                     | 0.40              |
| 2:C:884:VAL:HG11 | 2:C:1050:VAL:HG11 | 2.02                     | 0.40              |
| 2:C:1120:ALA:HB2 | 2:C:1199:LEU:HD23 | 2.03                     | 0.40              |
| 3:D:130:MET:HB3  | 3:D:135:ILE:HD11  | 2.03                     | 0.40              |
| 5:M:196:ARG:HH21 | 5:M:196:ARG:HB3   | 1.86                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:M:219:ILE:O    | 5:M:219:ILE:HG22  | 2.21                     | 0.40              |
| 7:T:14:DC:H2"    | 7:T:15:DA:C8      | 2.56                     | 0.40              |
| 1:B:97:GLU:HB2   | 1:B:147:GLN:HG3   | 2.04                     | 0.40              |
| 2:C:1072:ASN:OD1 | 2:C:1072:ASN:N    | 2.51                     | 0.40              |
| 3:D:343:LEU:HD13 | 3:D:343:LEU:HA    | 1.87                     | 0.40              |
| 5:M:147:ALA:HB1  | 5:M:156:ILE:CD1   | 2.51                     | 0.40              |
| 5:M:185:PHE:HB3  | 5:M:186:ASP:H     | 1.55                     | 0.40              |
| 5:M:277:LEU:HB2  | 5:M:278:VAL:H     | 1.76                     | 0.40              |
| 2:C:695:ALA:HB1  | 2:C:795:ALA:HB3   | 2.03                     | 0.40              |
| 2:C:901:LEU:HD11 | 2:C:905:ILE:HD11  | 2.02                     | 0.40              |
| 3:D:450:HIS:HE1  | 3:D:452:LEU:HD12  | 1.87                     | 0.40              |
| 5:M:168:ASP:OD1  | 5:M:168:ASP:N     | 2.55                     | 0.40              |
| 5:M:279:ARG:NH2  | 5:M:281:VAL:HB    | 2.37                     | 0.40              |
| 7:T:6:DT:H2"     | 7:T:7:DG:N7       | 2.37                     | 0.40              |
| 2:C:491:ASP:OD1  | 2:C:491:ASP:N     | 2.55                     | 0.40              |
| 2:C:700:VAL:HG13 | 2:C:1117:LEU:HD23 | 2.04                     | 0.40              |
| 2:C:902:LEU:CD2  | 2:C:910:ALA:HB2   | 2.48                     | 0.40              |
| 3:D:1328:THR:OG1 | 3:D:1329:THR:N    | 2.55                     | 0.40              |
| 5:M:46:LEU:H     | 5:M:46:LEU:HG     | 1.65                     | 0.40              |
| 5:M:227:LEU:HD13 | 5:M:227:LEU:O     | 2.19                     | 0.40              |
| 6:N:-13:DC:N4    | 7:T:13:DG:H1      | 2.06                     | 0.40              |
| 1:A:31:LEU:HD21  | 1:A:200:LYS:HA    | 2.03                     | 0.40              |
| 2:C:201:ARG:HG2  | 2:C:202:ARG:H     | 1.86                     | 0.40              |
| 2:C:1120:ALA:HB1 | 2:C:1198:LEU:HG   | 2.02                     | 0.40              |
| 3:D:370:LYS:HG2  | 3:D:441:LEU:HD23  | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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     | 305/329 (93%) | 283 (93%) | 22 (7%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 1   | B     | 218/329 (66%)    | 207 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| 2   | C     | 1339/1342 (100%) | 1239 (92%) | 89 (7%)  | 11 (1%)  | 16          | 44  |
| 3   | D     | 1322/1407 (94%)  | 1228 (93%) | 94 (7%)  | 0        | 100         | 100 |
| 4   | E     | 72/91 (79%)      | 71 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 5   | M     | 399/497 (80%)    | 330 (83%)  | 52 (13%) | 17 (4%)  | 2           | 13  |
| All | All   | 3655/3995 (92%)  | 3358 (92%) | 269 (7%) | 28 (1%)  | 18          | 44  |

All (28) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 1043 | ALA  |
| 2   | C     | 1044 | PRO  |
| 5   | M     | 18   | GLN  |
| 5   | M     | 120  | LEU  |
| 5   | M     | 195  | LEU  |
| 5   | M     | 287  | VAL  |
| 5   | M     | 288  | GLU  |
| 2   | C     | 922  | ASN  |
| 2   | C     | 1050 | VAL  |
| 5   | M     | 111  | VAL  |
| 5   | M     | 275  | ASP  |
| 5   | M     | 296  | ARG  |
| 5   | M     | 405  | SER  |
| 5   | M     | 407  | VAL  |
| 2   | C     | 897  | PRO  |
| 2   | C     | 1005 | GLU  |
| 5   | M     | 17   | PRO  |
| 2   | C     | 895  | LEU  |
| 2   | C     | 1003 | THR  |
| 5   | M     | 291  | ALA  |
| 2   | C     | 847  | PRO  |
| 2   | C     | 919  | ARG  |
| 5   | M     | 119  | THR  |
| 5   | M     | 193  | LYS  |
| 2   | C     | 993  | PRO  |
| 5   | M     | 152  | GLY  |
| 5   | M     | 259  | ARG  |
| 5   | M     | 269  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 248/286 (87%)   | 238 (96%)  | 10 (4%)   | 28          | 53 |
| 1   | B     | 180/286 (63%)   | 164 (91%)  | 16 (9%)   | 9           | 31 |
| 2   | C     | 1047/1157 (90%) | 905 (86%)  | 142 (14%) | 3           | 15 |
| 3   | D     | 913/1168 (78%)  | 881 (96%)  | 32 (4%)   | 32          | 56 |
| 4   | E     | 53/75 (71%)     | 52 (98%)   | 1 (2%)    | 50          | 66 |
| 5   | M     | 350/440 (80%)   | 238 (68%)  | 112 (32%) | 0           | 0  |
| All | All   | 2791/3412 (82%) | 2478 (89%) | 313 (11%) | 8           | 21 |

All (313) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | THR  |
| 1   | A     | 110 | VAL  |
| 1   | A     | 115 | ILE  |
| 1   | A     | 171 | LEU  |
| 1   | A     | 180 | VAL  |
| 1   | A     | 201 | LEU  |
| 1   | A     | 202 | VAL  |
| 1   | A     | 207 | THR  |
| 1   | A     | 262 | LEU  |
| 1   | A     | 289 | LEU  |
| 1   | B     | 10  | LYS  |
| 1   | B     | 14  | VAL  |
| 1   | B     | 16  | ILE  |
| 1   | B     | 29  | GLU  |
| 1   | B     | 33  | ARG  |
| 1   | B     | 65  | LEU  |
| 1   | B     | 78  | ILE  |
| 1   | B     | 133 | LEU  |
| 1   | B     | 144 | ILE  |
| 1   | B     | 145 | LYS  |
| 1   | B     | 150 | ARG  |
| 1   | B     | 153 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 182 | ARG  |
| 1   | B     | 196 | THR  |
| 1   | B     | 224 | LEU  |
| 1   | B     | 228 | LEU  |
| 2   | C     | 28  | LEU  |
| 2   | C     | 30  | ILE  |
| 2   | C     | 37  | LYS  |
| 2   | C     | 49  | LEU  |
| 2   | C     | 164 | THR  |
| 2   | C     | 171 | LEU  |
| 2   | C     | 176 | ILE  |
| 2   | C     | 196 | VAL  |
| 2   | C     | 208 | ILE  |
| 2   | C     | 209 | ILE  |
| 2   | C     | 210 | LEU  |
| 2   | C     | 214 | ASN  |
| 2   | C     | 221 | LEU  |
| 2   | C     | 228 | VAL  |
| 2   | C     | 229 | ILE  |
| 2   | C     | 261 | VAL  |
| 2   | C     | 302 | ILE  |
| 2   | C     | 310 | ILE  |
| 2   | C     | 324 | LYS  |
| 2   | C     | 353 | VAL  |
| 2   | C     | 397 | LEU  |
| 2   | C     | 414 | ILE  |
| 2   | C     | 487 | LEU  |
| 2   | C     | 488 | MET  |
| 2   | C     | 490 | GLN  |
| 2   | C     | 503 | LYS  |
| 2   | C     | 538 | LEU  |
| 2   | C     | 542 | ARG  |
| 2   | C     | 589 | THR  |
| 2   | C     | 603 | ILE  |
| 2   | C     | 677 | ASN  |
| 2   | C     | 697 | LYS  |
| 2   | C     | 748 | ILE  |
| 2   | C     | 755 | LYS  |
| 2   | C     | 761 | GLN  |
| 2   | C     | 783 | LEU  |
| 2   | C     | 800 | MET  |
| 2   | C     | 830 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 831 | ILE  |
| 2   | C     | 833 | ILE  |
| 2   | C     | 834 | GLN  |
| 2   | C     | 835 | GLU  |
| 2   | C     | 836 | LEU  |
| 2   | C     | 838 | CYS  |
| 2   | C     | 840 | SER  |
| 2   | C     | 841 | ARG  |
| 2   | C     | 842 | ASP  |
| 2   | C     | 843 | THR  |
| 2   | C     | 844 | LYS  |
| 2   | C     | 845 | LEU  |
| 2   | C     | 848 | GLU  |
| 2   | C     | 850 | ILE  |
| 2   | C     | 854 | ILE  |
| 2   | C     | 856 | ASN  |
| 2   | C     | 862 | LEU  |
| 2   | C     | 864 | LYS  |
| 2   | C     | 865 | LEU  |
| 2   | C     | 868 | SER  |
| 2   | C     | 870 | ILE  |
| 2   | C     | 873 | ILE  |
| 2   | C     | 881 | ASP  |
| 2   | C     | 882 | ILE  |
| 2   | C     | 886 | LYS  |
| 2   | C     | 887 | VAL  |
| 2   | C     | 890 | LYS  |
| 2   | C     | 895 | LEU  |
| 2   | C     | 901 | LEU  |
| 2   | C     | 902 | LEU  |
| 2   | C     | 903 | ARG  |
| 2   | C     | 913 | VAL  |
| 2   | C     | 915 | ASP  |
| 2   | C     | 917 | SER  |
| 2   | C     | 918 | LEU  |
| 2   | C     | 919 | ARG  |
| 2   | C     | 922 | ASN  |
| 2   | C     | 925 | SER  |
| 2   | C     | 927 | THR  |
| 2   | C     | 928 | VAL  |
| 2   | C     | 929 | ILE  |
| 2   | C     | 931 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 932  | GLN  |
| 2   | C     | 933  | VAL  |
| 2   | C     | 936  | ARG  |
| 2   | C     | 937  | ASP  |
| 2   | C     | 939  | VAL  |
| 2   | C     | 940  | GLU  |
| 2   | C     | 944  | ARG  |
| 2   | C     | 946  | LEU  |
| 2   | C     | 948  | ILE  |
| 2   | C     | 953  | LEU  |
| 2   | C     | 954  | LYS  |
| 2   | C     | 955  | GLN  |
| 2   | C     | 957  | LYS  |
| 2   | C     | 958  | LYS  |
| 2   | C     | 959  | ASP  |
| 2   | C     | 962  | GLU  |
| 2   | C     | 964  | LEU  |
| 2   | C     | 966  | ILE  |
| 2   | C     | 971  | LEU  |
| 2   | C     | 974  | ARG  |
| 2   | C     | 975  | ILE  |
| 2   | C     | 978  | VAL  |
| 2   | C     | 979  | LEU  |
| 2   | C     | 984  | VAL  |
| 2   | C     | 992  | LEU  |
| 2   | C     | 995  | ASP  |
| 2   | C     | 1006 | GLU  |
| 2   | C     | 1011 | LEU  |
| 2   | C     | 1014 | LEU  |
| 2   | C     | 1016 | GLU  |
| 2   | C     | 1017 | GLN  |
| 2   | C     | 1021 | LEU  |
| 2   | C     | 1022 | LYS  |
| 2   | C     | 1024 | GLU  |
| 2   | C     | 1028 | LYS  |
| 2   | C     | 1029 | LEU  |
| 2   | C     | 1032 | LYS  |
| 2   | C     | 1035 | LYS  |
| 2   | C     | 1036 | ILE  |
| 2   | C     | 1038 | GLN  |
| 2   | C     | 1040 | ASP  |
| 2   | C     | 1042 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 1046 | VAL  |
| 2   | C     | 1047 | LEU  |
| 2   | C     | 1048 | LYS  |
| 2   | C     | 1049 | ILE  |
| 2   | C     | 1051 | LYS  |
| 2   | C     | 1052 | VAL  |
| 2   | C     | 1054 | LEU  |
| 2   | C     | 1056 | VAL  |
| 2   | C     | 1057 | LYS  |
| 2   | C     | 1058 | ARG  |
| 2   | C     | 1059 | ARG  |
| 2   | C     | 1119 | MET  |
| 2   | C     | 1140 | LYS  |
| 2   | C     | 1161 | LEU  |
| 2   | C     | 1166 | ASP  |
| 2   | C     | 1210 | ILE  |
| 2   | C     | 1237 | HIS  |
| 2   | C     | 1250 | SER  |
| 2   | C     | 1251 | TYR  |
| 2   | C     | 1303 | LYS  |
| 3   | D     | 50   | LYS  |
| 3   | D     | 72   | CYS  |
| 3   | D     | 74   | LYS  |
| 3   | D     | 76   | LYS  |
| 3   | D     | 161  | THR  |
| 3   | D     | 166  | LEU  |
| 3   | D     | 223  | LEU  |
| 3   | D     | 245  | LEU  |
| 3   | D     | 274  | ASN  |
| 3   | D     | 321  | LYS  |
| 3   | D     | 325  | LYS  |
| 3   | D     | 342  | LEU  |
| 3   | D     | 343  | LEU  |
| 3   | D     | 346  | ARG  |
| 3   | D     | 363  | LEU  |
| 3   | D     | 395  | LYS  |
| 3   | D     | 428  | THR  |
| 3   | D     | 518  | VAL  |
| 3   | D     | 552  | ILE  |
| 3   | D     | 649  | LYS  |
| 3   | D     | 695  | LYS  |
| 3   | D     | 698  | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 821  | MET  |
| 3   | D     | 831  | VAL  |
| 3   | D     | 842  | ARG  |
| 3   | D     | 885  | VAL  |
| 3   | D     | 901  | ARG  |
| 3   | D     | 930  | LEU  |
| 3   | D     | 1159 | ILE  |
| 3   | D     | 1240 | VAL  |
| 3   | D     | 1247 | LYS  |
| 3   | D     | 1266 | ILE  |
| 4   | E     | 21   | LEU  |
| 5   | M     | 18   | GLN  |
| 5   | M     | 19   | LEU  |
| 5   | M     | 20   | GLN  |
| 5   | M     | 23   | ILE  |
| 5   | M     | 24   | ARG  |
| 5   | M     | 25   | LEU  |
| 5   | M     | 26   | LEU  |
| 5   | M     | 28   | LEU  |
| 5   | M     | 33   | LEU  |
| 5   | M     | 41   | LEU  |
| 5   | M     | 42   | GLU  |
| 5   | M     | 113  | GLN  |
| 5   | M     | 115  | GLU  |
| 5   | M     | 117  | THR  |
| 5   | M     | 120  | LEU  |
| 5   | M     | 121  | GLN  |
| 5   | M     | 124  | LEU  |
| 5   | M     | 125  | MET  |
| 5   | M     | 130  | LEU  |
| 5   | M     | 134  | THR  |
| 5   | M     | 138  | ARG  |
| 5   | M     | 143  | SER  |
| 5   | M     | 144  | ILE  |
| 5   | M     | 145  | VAL  |
| 5   | M     | 146  | ASP  |
| 5   | M     | 148  | VAL  |
| 5   | M     | 149  | ASP  |
| 5   | M     | 150  | ASP  |
| 5   | M     | 151  | THR  |
| 5   | M     | 153  | TYR  |
| 5   | M     | 156  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | M     | 157 | GLN  |
| 5   | M     | 172 | LEU  |
| 5   | M     | 173 | GLU  |
| 5   | M     | 176 | GLU  |
| 5   | M     | 180 | LYS  |
| 5   | M     | 181 | ARG  |
| 5   | M     | 184 | ARG  |
| 5   | M     | 185 | PHE  |
| 5   | M     | 188 | VAL  |
| 5   | M     | 193 | LYS  |
| 5   | M     | 196 | ARG  |
| 5   | M     | 197 | ASP  |
| 5   | M     | 199 | LEU  |
| 5   | M     | 201 | ILE  |
| 5   | M     | 215 | GLU  |
| 5   | M     | 217 | ARG  |
| 5   | M     | 218 | LEU  |
| 5   | M     | 219 | ILE  |
| 5   | M     | 220 | ILE  |
| 5   | M     | 224 | LEU  |
| 5   | M     | 225 | ASP  |
| 5   | M     | 226 | LEU  |
| 5   | M     | 245 | VAL  |
| 5   | M     | 252 | LEU  |
| 5   | M     | 254 | GLN  |
| 5   | M     | 259 | ARG  |
| 5   | M     | 264 | ILE  |
| 5   | M     | 265 | GLN  |
| 5   | M     | 266 | THR  |
| 5   | M     | 267 | SER  |
| 5   | M     | 270 | GLU  |
| 5   | M     | 271 | TYR  |
| 5   | M     | 272 | VAL  |
| 5   | M     | 273 | ILE  |
| 5   | M     | 275 | ASP  |
| 5   | M     | 276 | VAL  |
| 5   | M     | 277 | LEU  |
| 5   | M     | 279 | ARG  |
| 5   | M     | 280 | LYS  |
| 5   | M     | 287 | VAL  |
| 5   | M     | 288 | GLU  |
| 5   | M     | 289 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | M     | 293 | SER  |
| 5   | M     | 294 | ILE  |
| 5   | M     | 297 | LEU  |
| 5   | M     | 299 | ILE  |
| 5   | M     | 323 | LEU  |
| 5   | M     | 329 | LEU  |
| 5   | M     | 331 | LYS  |
| 5   | M     | 335 | SER  |
| 5   | M     | 336 | ARG  |
| 5   | M     | 338 | ASP  |
| 5   | M     | 340 | LEU  |
| 5   | M     | 341 | LEU  |
| 5   | M     | 342 | ARG  |
| 5   | M     | 343 | VAL  |
| 5   | M     | 344 | SER  |
| 5   | M     | 345 | ARG  |
| 5   | M     | 347 | ILE  |
| 5   | M     | 350 | GLN  |
| 5   | M     | 375 | GLU  |
| 5   | M     | 378 | GLU  |
| 5   | M     | 379 | SER  |
| 5   | M     | 383 | ARG  |
| 5   | M     | 386 | THR  |
| 5   | M     | 387 | GLN  |
| 5   | M     | 390 | LEU  |
| 5   | M     | 391 | HIS  |
| 5   | M     | 394 | ARG  |
| 5   | M     | 398 | GLU  |
| 5   | M     | 399 | LEU  |
| 5   | M     | 400 | LYS  |
| 5   | M     | 405 | SER  |
| 5   | M     | 408 | ASN  |
| 5   | M     | 423 | LEU  |
| 5   | M     | 435 | LYS  |
| 5   | M     | 452 | MET  |
| 5   | M     | 455 | ARG  |
| 5   | M     | 456 | ARG  |
| 5   | M     | 460 | LYS  |
| 5   | M     | 474 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 84   | ASN  |
| 1   | A     | 186  | ASN  |
| 1   | B     | 37   | HIS  |
| 1   | B     | 128  | HIS  |
| 2   | C     | 357  | ASN  |
| 2   | C     | 490  | GLN  |
| 2   | C     | 526  | HIS  |
| 2   | C     | 573  | ASN  |
| 2   | C     | 808  | ASN  |
| 2   | C     | 834  | GLN  |
| 2   | C     | 932  | GLN  |
| 2   | C     | 955  | GLN  |
| 2   | C     | 1017 | GLN  |
| 2   | C     | 1038 | GLN  |
| 2   | C     | 1175 | ASN  |
| 2   | C     | 1313 | HIS  |
| 3   | D     | 45   | ASN  |
| 3   | D     | 419  | HIS  |
| 3   | D     | 477  | GLN  |
| 3   | D     | 875  | ASN  |
| 5   | M     | 27   | GLN  |
| 5   | M     | 34   | GLN  |
| 5   | M     | 39   | GLN  |
| 5   | M     | 127  | GLN  |
| 5   | M     | 205  | GLN  |
| 5   | M     | 322  | ASN  |
| 5   | M     | 351  | GLN  |
| 5   | M     | 387  | GLN  |
| 5   | M     | 406  | HIS  |
| 5   | M     | 408  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

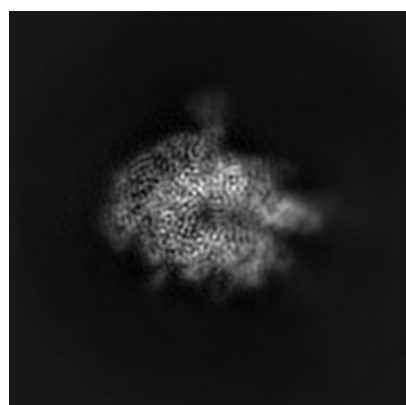
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14200. These allow visual inspection of the internal detail of the map and identification of artifacts.

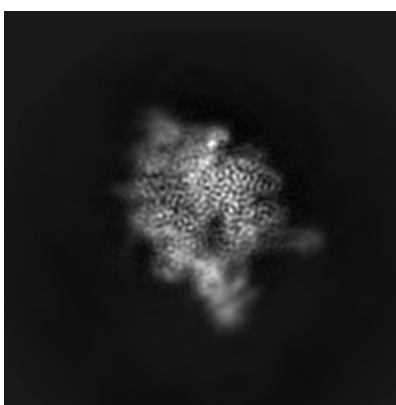
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

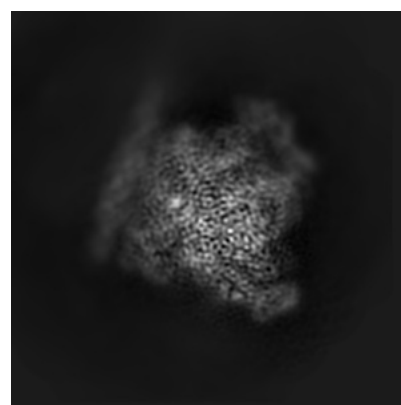
#### 6.1.1 Primary map



X



Y

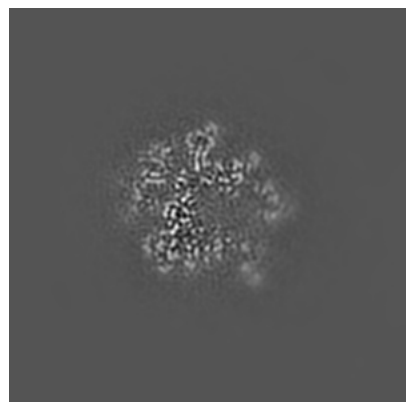


Z

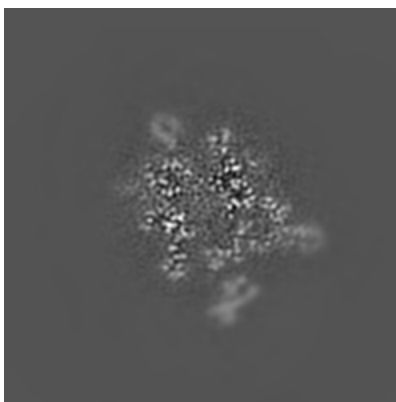
The images above show the map projected in three orthogonal directions.

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

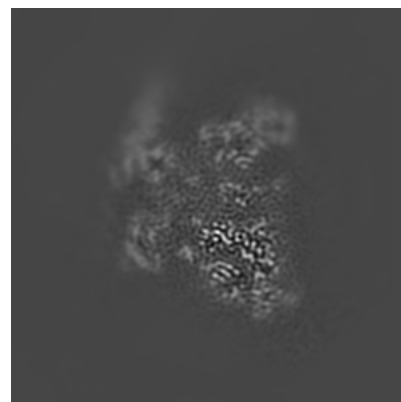
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

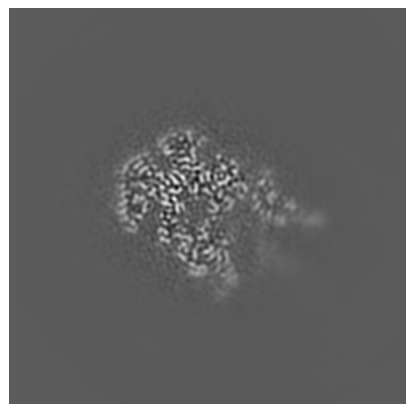


Z Index: 128

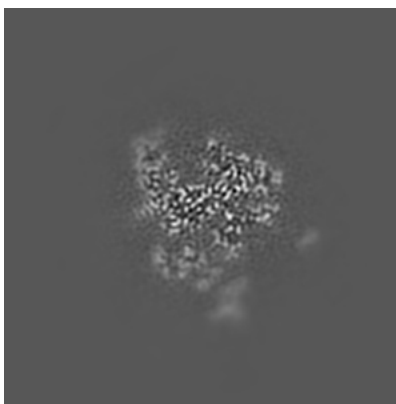
The images above show central slices of the map in three orthogonal directions.

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

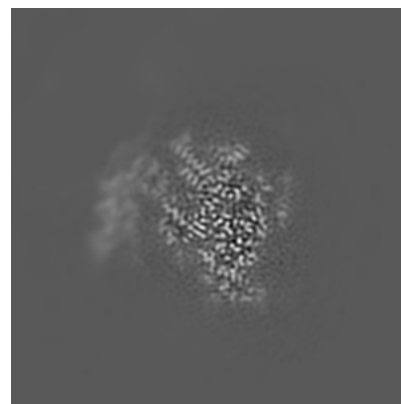
### 6.3.1 Primary map



X Index: 145



Y Index: 115

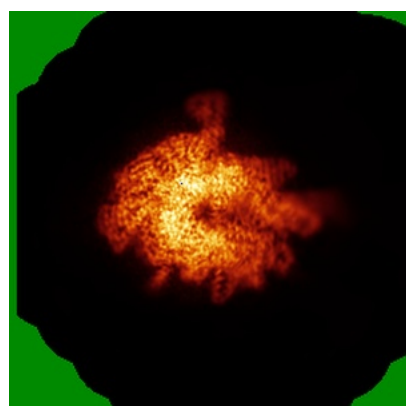


Z Index: 144

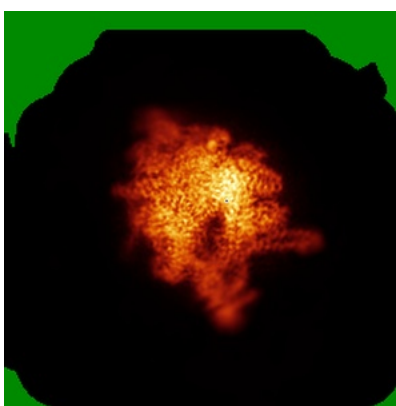
The images above show the largest variance slices of the map in three orthogonal directions.

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

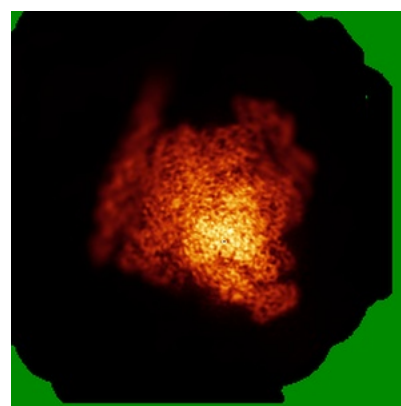
### 6.4.1 Primary map



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.

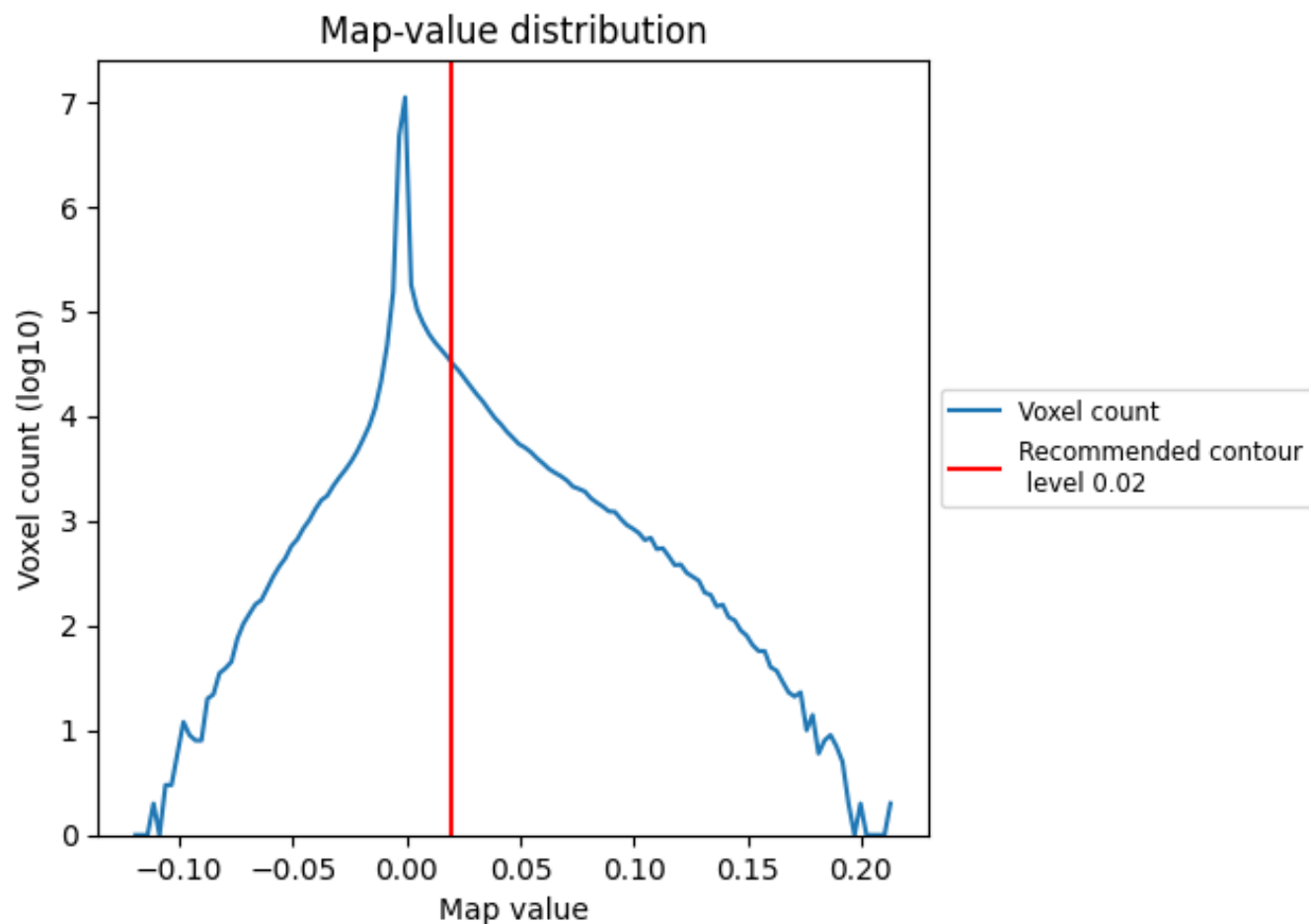
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

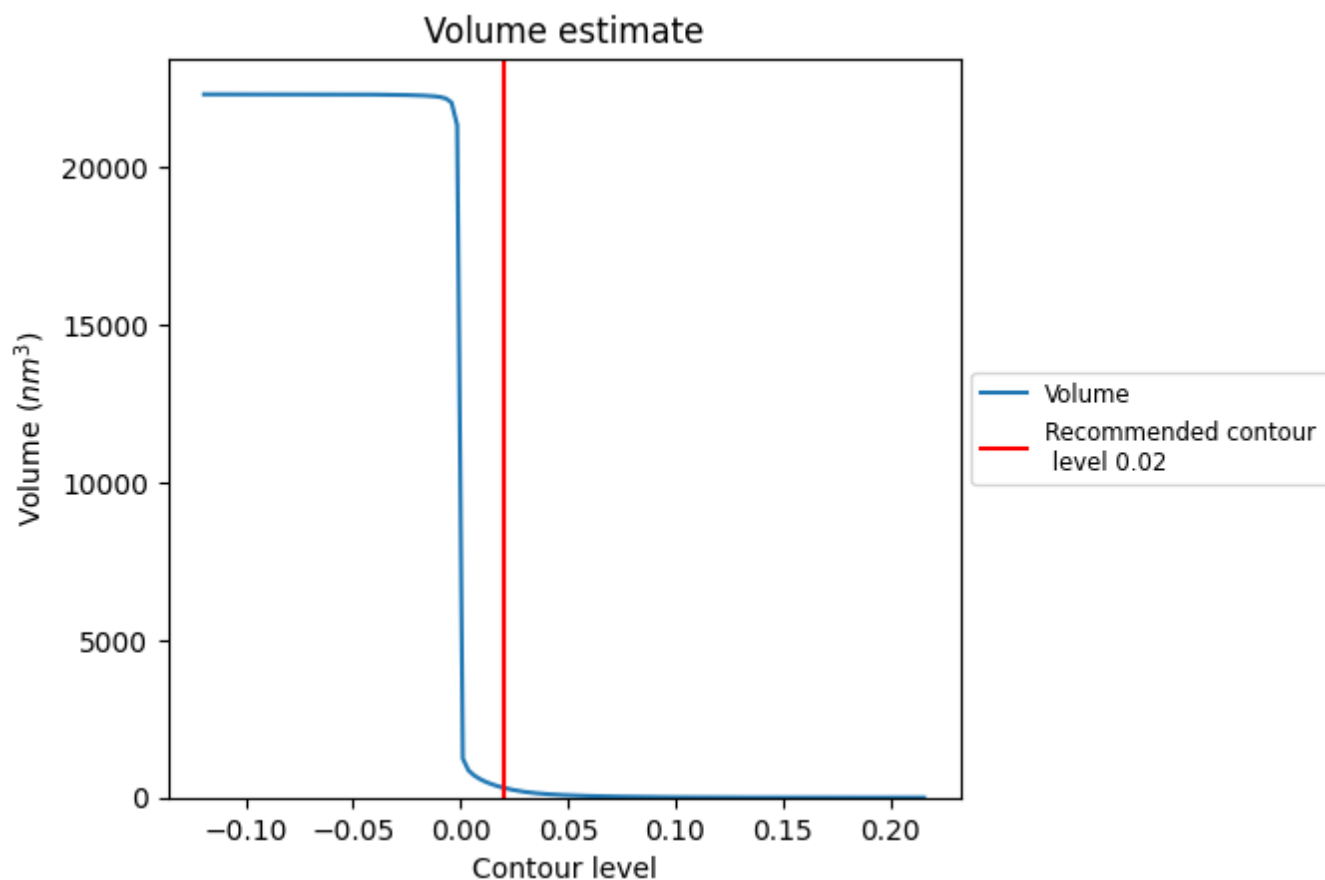
This section contains the results of statistical analysis of the map.

### 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.

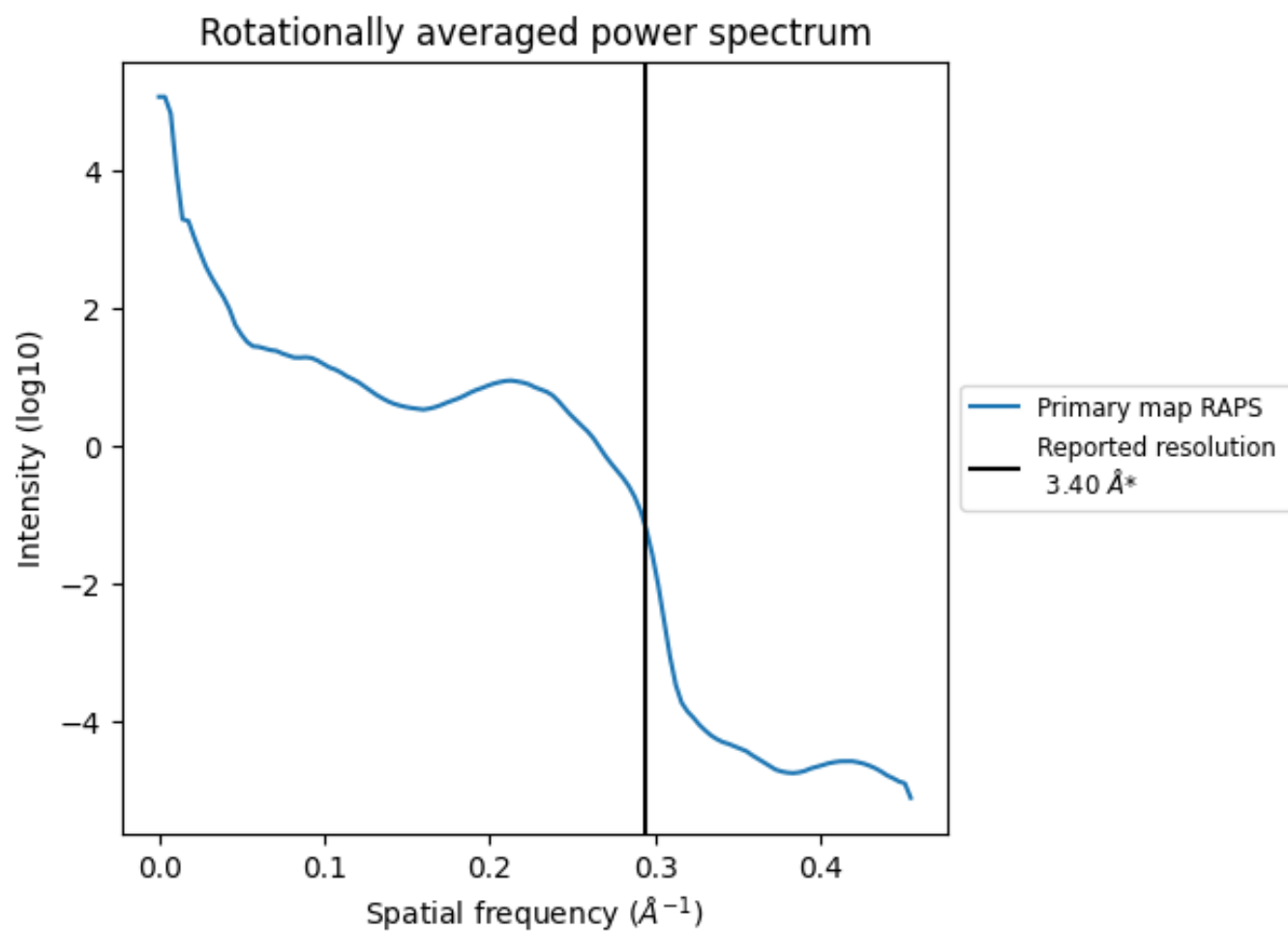
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 312  $\text{nm}^3$ ; this corresponds to an approximate mass of 281 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 0.294 Å<sup>-1</sup>

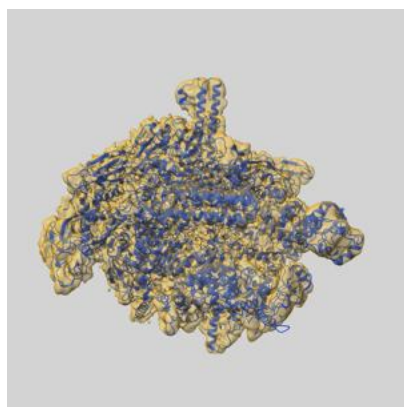
## 8 Fourier-Shell correlation

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

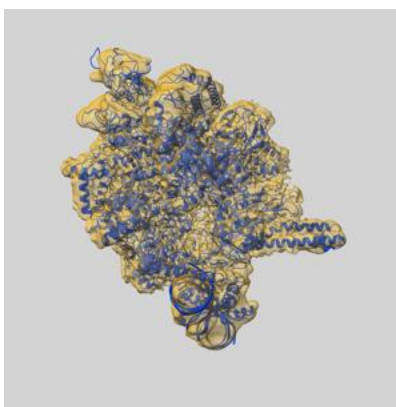
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14200 and PDB model 7QXI. Per-residue inclusion information can be found in section [3](#) on page [6](#).

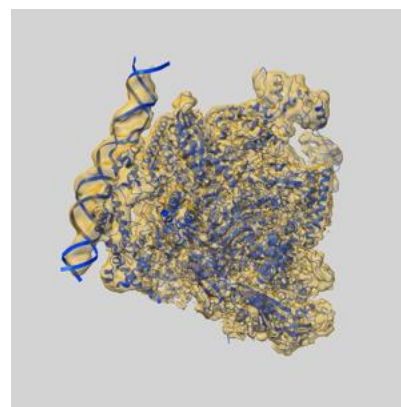
### 9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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](#)



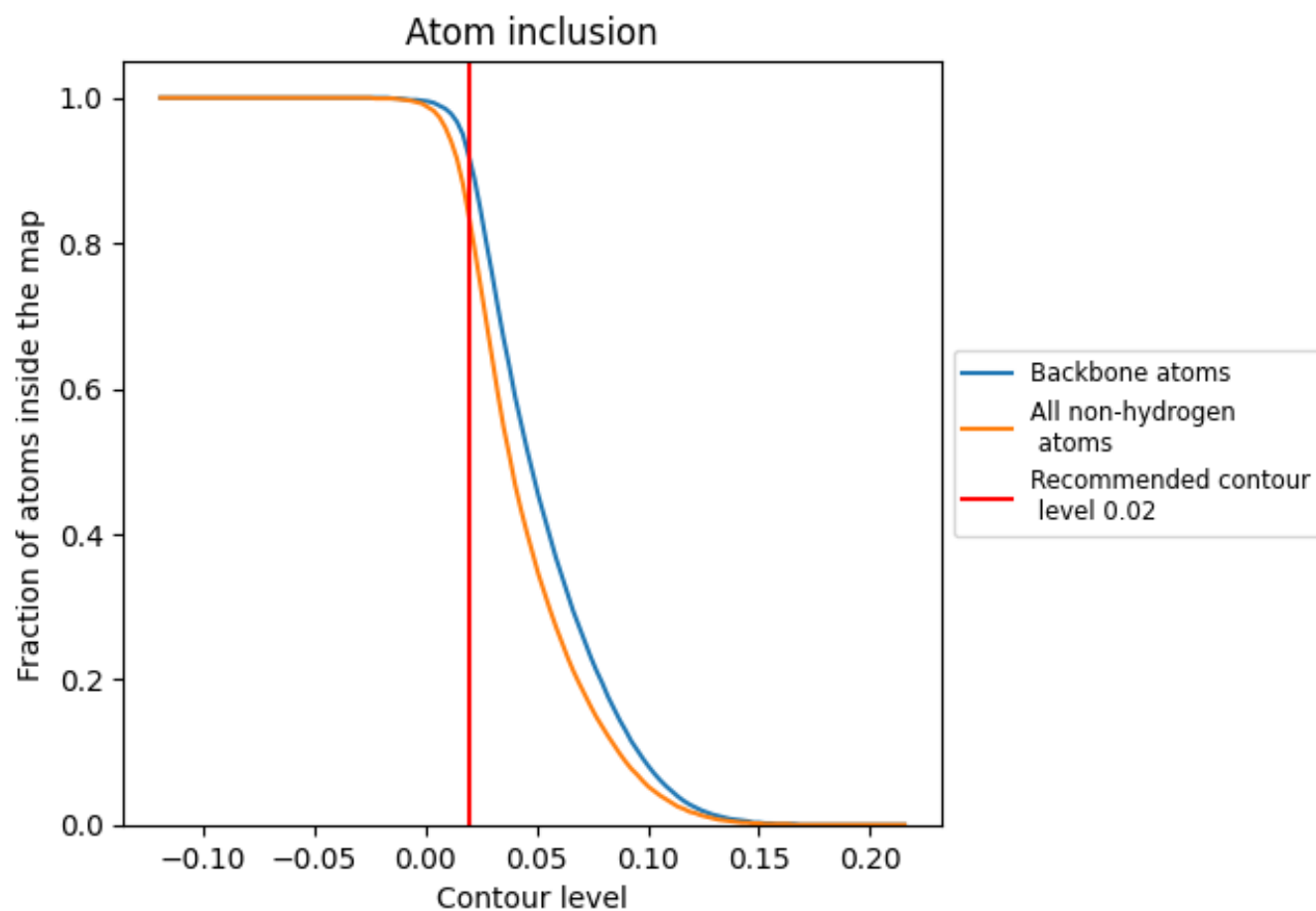
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 91% of all backbone atoms, 83% 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></div></div> 0.8290 | <div><div></div></div> 0.3640 |
| A     | <div><div></div></div> 0.7870 | <div><div></div></div> 0.3820 |
| B     | <div><div></div></div> 0.8450 | <div><div></div></div> 0.3680 |
| C     | <div><div></div></div> 0.8610 | <div><div></div></div> 0.4040 |
| D     | <div><div></div></div> 0.8310 | <div><div></div></div> 0.3630 |
| E     | <div><div></div></div> 0.8770 | <div><div></div></div> 0.4130 |
| M     | <div><div></div></div> 0.7920 | <div><div></div></div> 0.3010 |
| N     | <div><div></div></div> 0.7470 | <div><div></div></div> 0.1710 |
| T     | <div><div></div></div> 0.6800 | <div><div></div></div> 0.1780 |

1.0

0.0

<0.0