



## Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 05:06 PM UTC

PDB ID : 3J1N / pdb\_00003j1n  
EMDB ID : EMD-5407  
Title : Cryo-EM map of a yeast minimal preinitiation complex interacting with the Mediator Head module  
Authors : Asturias, F.J.; Imasaki, T.  
Deposited on : 2012-03-29  
Resolution : 16.00 Å (reported)  
Based on initial model : 1WCM

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:

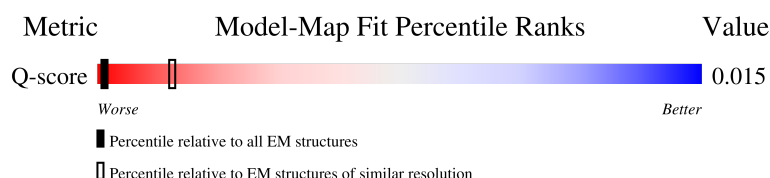
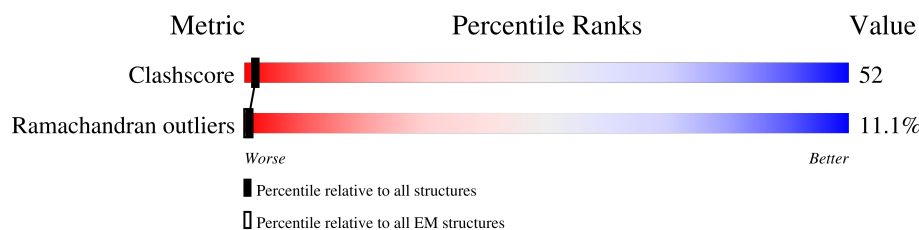
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 16.00 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                       | -                                                        |
| Q-score               | -                           | 25397                       | 41 ( 15.50 - 16.50 )                                     |

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     | 1455   |  |
| 2   | B     | 1224   |  |
| 3   | C     | 268    |  |
| 4   | D     | 218    |  |
| 5   | E     | 215    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 6   | F     | 84     |                  |
| 7   | G     | 171    |                  |
| 8   | H     | 146    |                  |
| 9   | I     | 122    |                  |
| 10  | J     | 70     |                  |
| 11  | K     | 120    |                  |
| 12  | L     | 70     |                  |

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 19237 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 II subunit RPB1.

| Mol | Chain | Residues | Atoms |      |      |      | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---------|-------|
| 1   | A     | 1412     | Total | C    | N    | O    | 0       | 0     |
|     |       |          | 6964  | 4140 | 1412 | 1412 |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

| Mol | Chain | Residues | Atoms |      |      |      | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---------|-------|
| 2   | B     | 1094     | Total | C    | N    | O    | 0       | 0     |
|     |       |          | 5397  | 3209 | 1094 | 1094 |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 3   | C     | 266      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1317  | 785 | 266 | 266 |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 4   | D     | 177      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 878   | 524 | 177 | 177 |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPABC1.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 5   | E     | 214      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1062  | 634 | 214 | 214 |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPABC2.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 6   | F     | 84       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 417   | 249 | 84 | 84 |         |       |

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 7   | G     | 171      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 841   | 499 | 171 | 171 |         |       |

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPABC3.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 8   | H     | 133      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 659   | 393 | 133 | 133 |         |       |

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 9   | I     | 118      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 587   | 351 | 118 | 118 |         |       |

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPABC5.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10  | J     | 65       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 321   | 191 | 65 | 65 |         |       |

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 11  | K     | 114      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 565   | 337 | 114 | 114 |         |       |

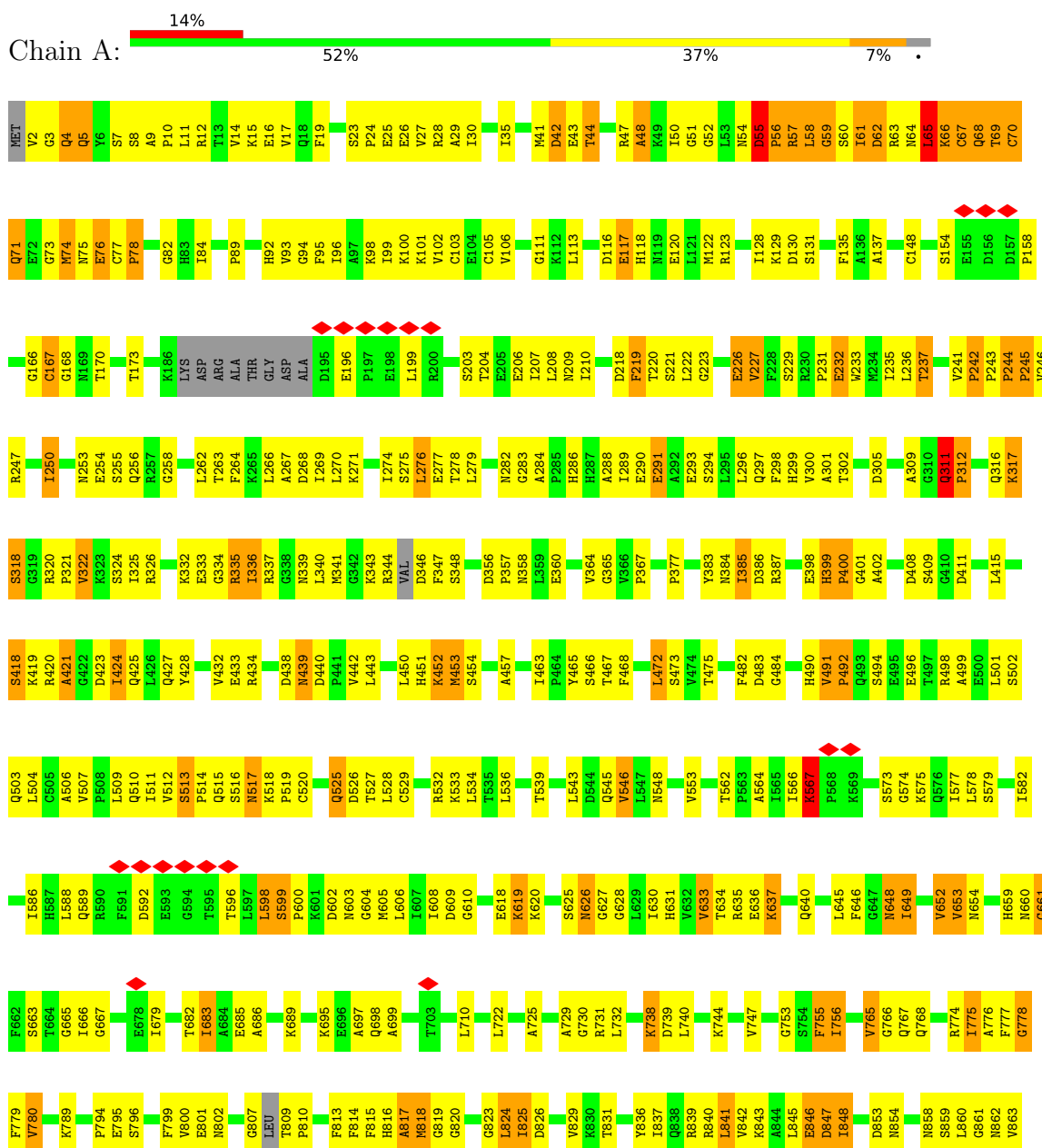
- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPABC4.

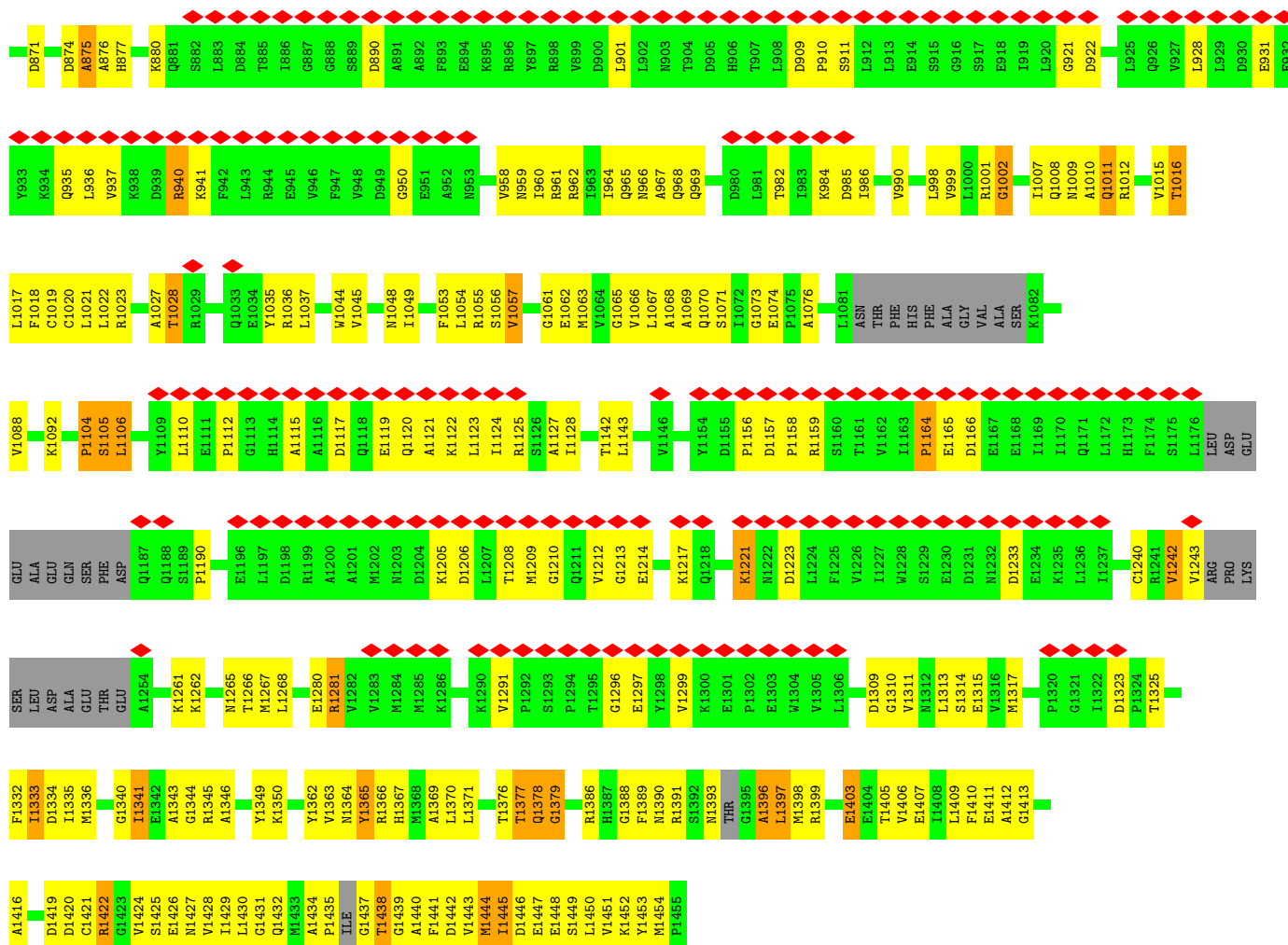
| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 12  | L     | 46       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 229   | 137 | 46 | 46 |         |       |

### 3 Residue-property plots

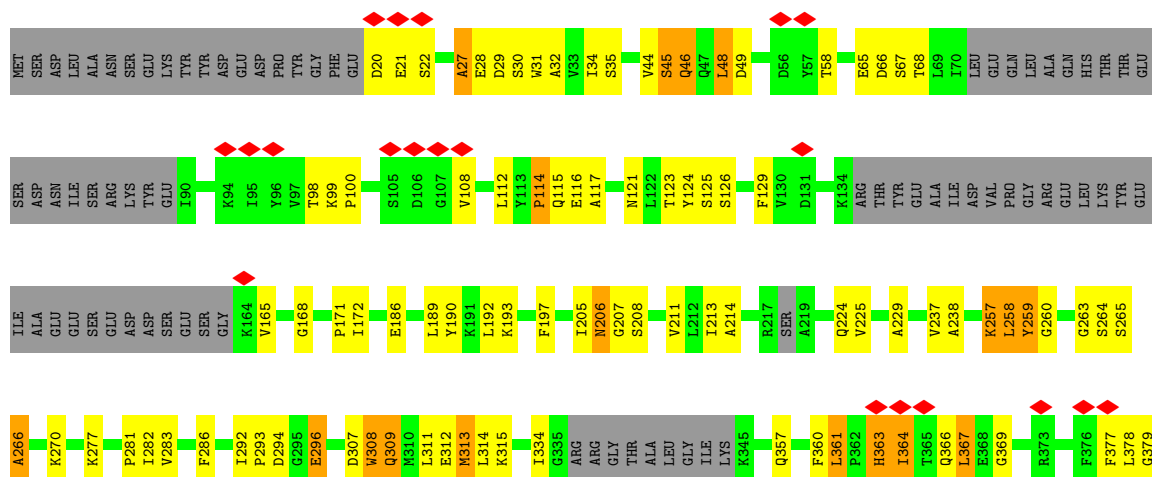
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

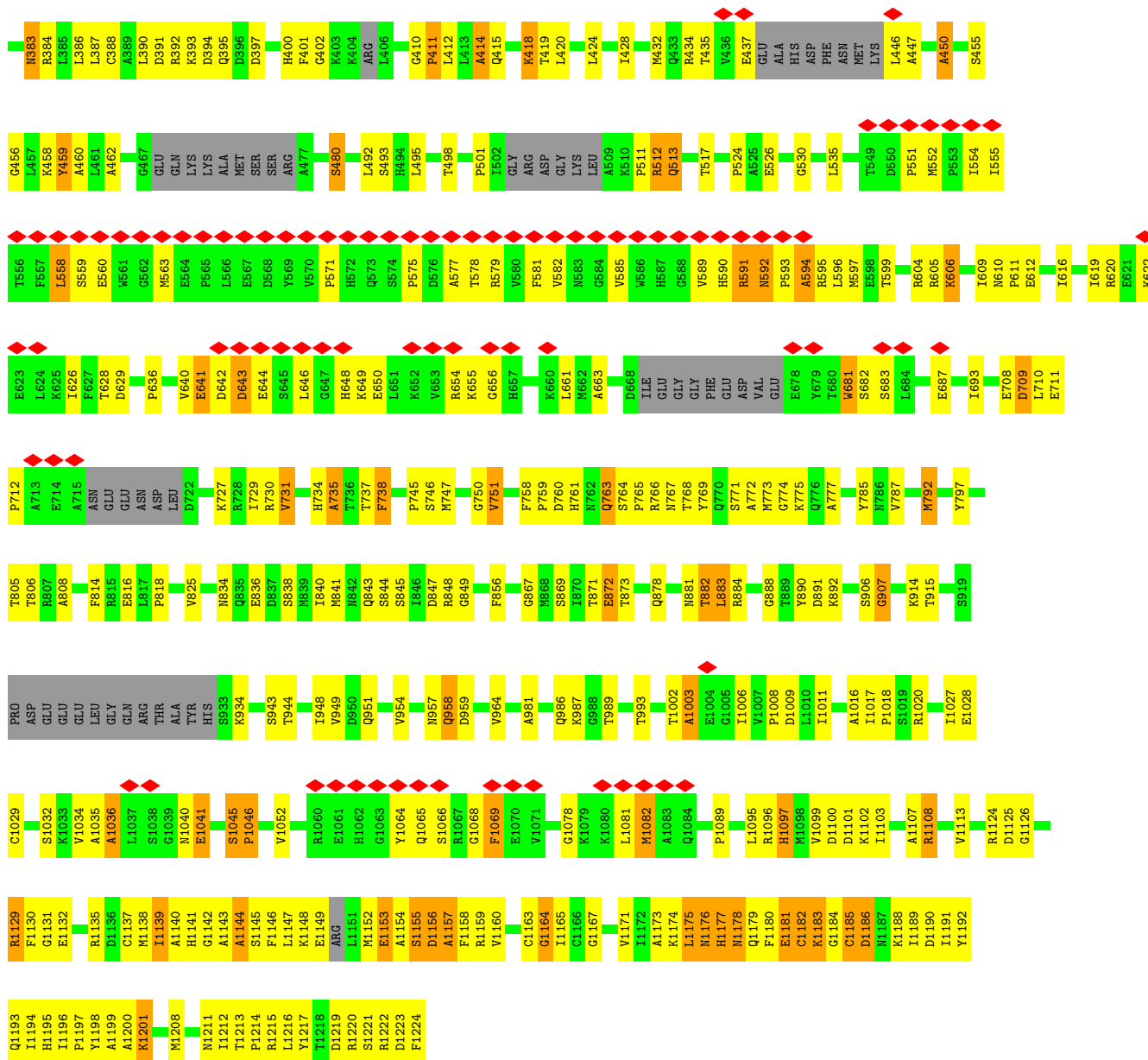
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



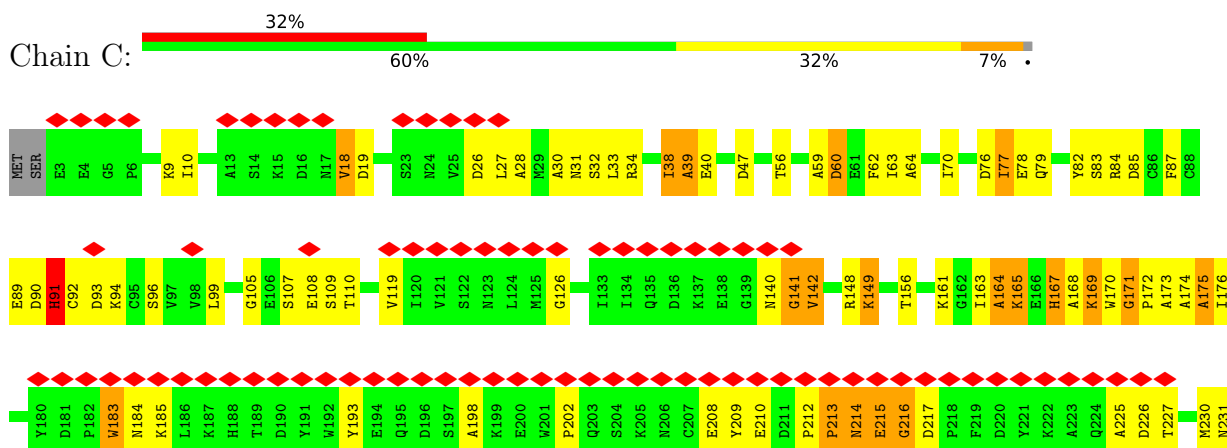


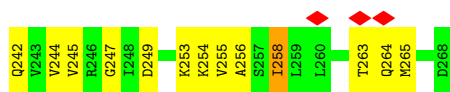
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2



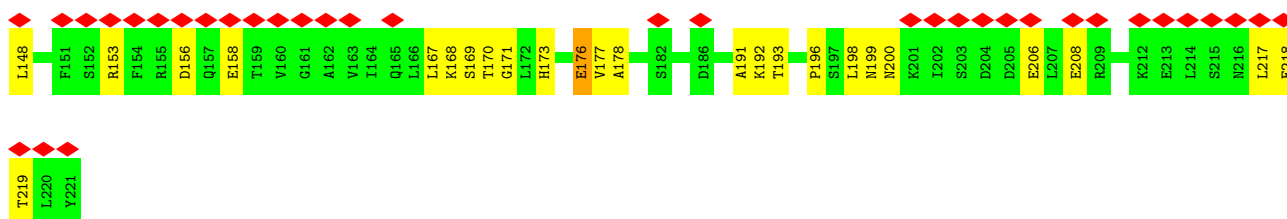
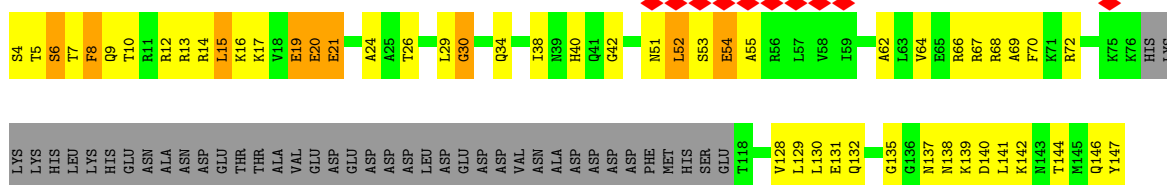


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

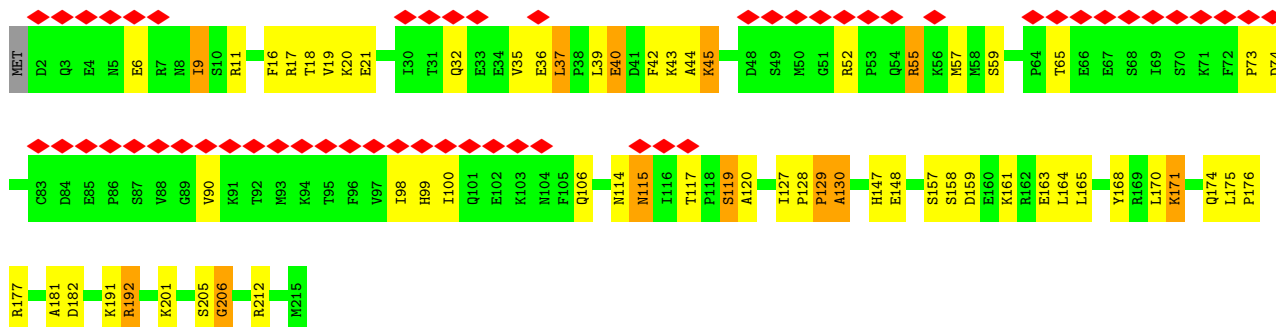




• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



• Molecule 5: DNA-directed RNA polymerase II subunit RPABC1

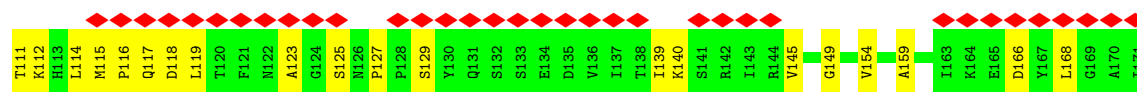


• Molecule 6: DNA-directed RNA polymerase II subunit RPABC2

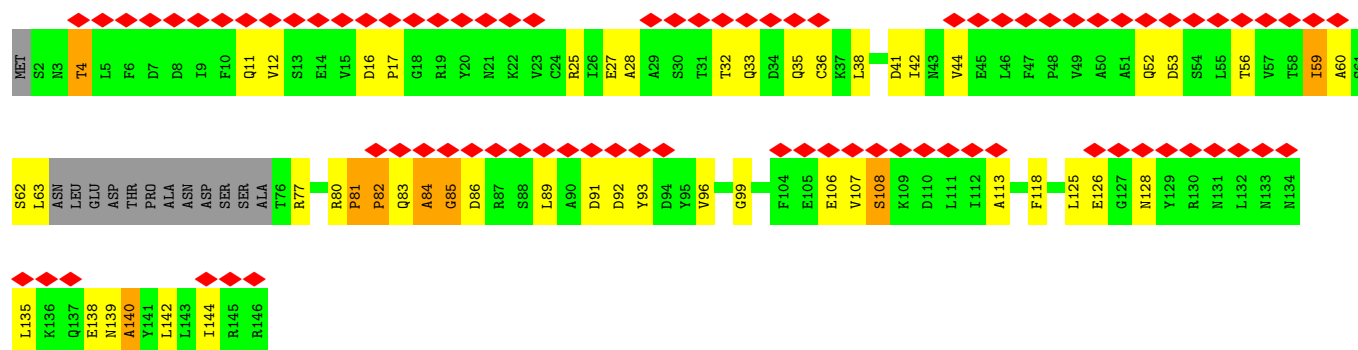


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

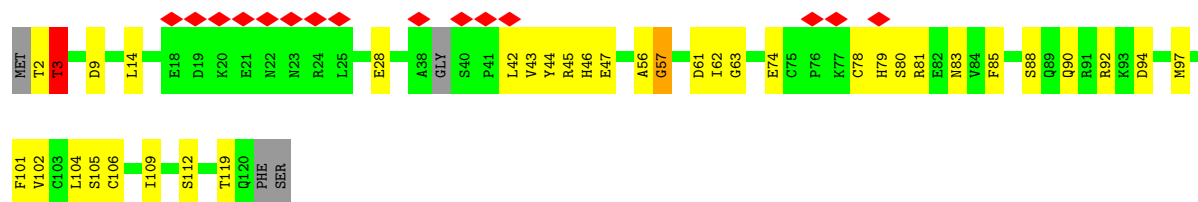




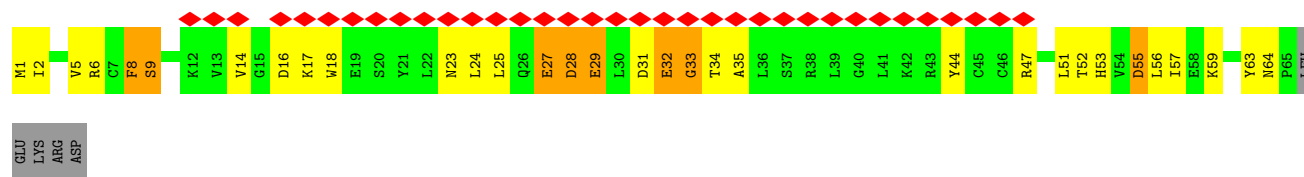
• Molecule 8: DNA-directed RNA polymerase II subunit RPABC3



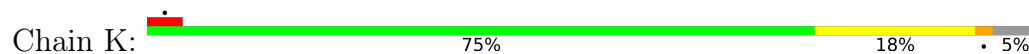
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

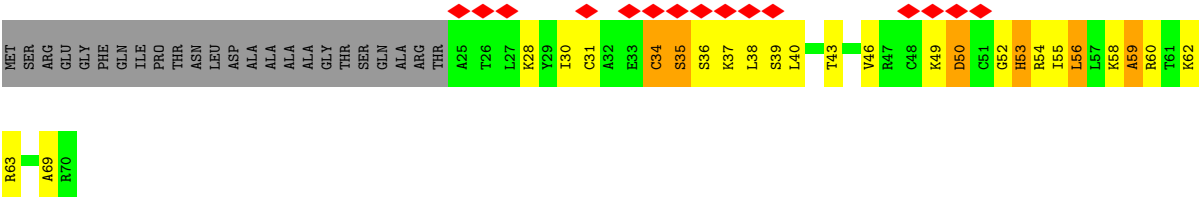


• Molecule 10: DNA-directed RNA polymerase II subunit RPABC5



• Molecule 11: DNA-directed RNA polymerase II subunit RPB11





## 4 Experimental information

| Property                             | Value                       | Source    |
|--------------------------------------|-----------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE             | Depositor |
| Imposed symmetry                     | POINT, C1                   | Depositor |
| Number of particles used             | 51000                       | Depositor |
| Resolution determination method      | FSC 0.5 CUT-OFF             | Depositor |
| CTF correction method                | Each CCD frame              | Depositor |
| Microscope                           | FEI TECNAI F20              | Depositor |
| Voltage (kV)                         | 120                         | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 10                          | Depositor |
| Minimum defocus (nm)                 | 800                         | Depositor |
| Maximum defocus (nm)                 | 3800                        | Depositor |
| Magnification                        | 50000                       | Depositor |
| Image detector                       | TVIPS TEMCAM-F415 (4k x 4k) | Depositor |
| Maximum map value                    | 32.476                      | Depositor |
| Minimum map value                    | -4.340                      | Depositor |
| Average map value                    | 0.557                       | Depositor |
| Map value standard deviation         | 2.374                       | Depositor |
| Recommended contour level            | 3.25                        | Depositor |
| Map size ( $\text{\AA}$ )            | 268.1, 268.1, 268.1         | wwPDB     |
| Map dimensions                       | 70, 70, 70                  | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0            | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 3.83, 3.83, 3.83            | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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     | 0.66         | 1/6953 (0.0%)  | 1.45        | 93/9659 (1.0%)   |
| 2   | B     | 0.62         | 0/5384         | 1.25        | 59/7473 (0.8%)   |
| 3   | C     | 0.71         | 0/1316         | 1.35        | 15/1833 (0.8%)   |
| 4   | D     | 0.57         | 0/876          | 1.39        | 13/1219 (1.1%)   |
| 5   | E     | 0.54         | 0/1061         | 1.20        | 10/1479 (0.7%)   |
| 6   | F     | 0.74         | 0/416          | 1.45        | 9/579 (1.6%)     |
| 7   | G     | 0.68         | 0/840          | 1.36        | 17/1166 (1.5%)   |
| 8   | H     | 0.53         | 0/657          | 1.25        | 7/913 (0.8%)     |
| 9   | I     | 0.69         | 0/585          | 2.66        | 13/814 (1.6%)    |
| 10  | J     | 0.69         | 0/320          | 1.30        | 1/444 (0.2%)     |
| 11  | K     | 0.62         | 0/564          | 1.26        | 3/785 (0.4%)     |
| 12  | L     | 0.78         | 0/228          | 1.25        | 2/317 (0.6%)     |
| All | All   | 0.64         | 1/19200 (0.0%) | 1.41        | 242/26681 (0.9%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 999 | VAL  | CA-CB | -5.38 | 1.50        | 1.55     |

All (242) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 9   | I     | 3    | THR  | O-C-N  | -50.59 | 42.06       | 123.00   |
| 1   | A     | 768  | GLN  | O-C-N  | -31.95 | 71.89       | 123.00   |
| 9   | I     | 3    | THR  | CA-C-N | -28.24 | 70.87       | 121.70   |
| 9   | I     | 3    | THR  | C-N-CA | -28.24 | 70.87       | 121.70   |
| 1   | A     | 65   | LEU  | CA-C-N | 28.03  | 172.16      | 121.70   |
| 1   | A     | 65   | LEU  | C-N-CA | 28.03  | 172.16      | 121.70   |
| 1   | A     | 65   | LEU  | O-C-N  | 21.59  | 157.55      | 123.00   |
| 1   | A     | 848  | ILE  | O-C-N  | 16.99  | 150.19      | 123.00   |
| 2   | B     | 1185 | CYS  | N-CA-C | -13.56 | 96.70       | 113.38   |
| 4   | D     | 54   | GLU  | N-CA-C | -13.27 | 97.59       | 114.04   |
| 1   | A     | 452  | LYS  | N-CA-C | -13.21 | 96.93       | 111.07   |

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| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 4   | D     | 26   | THR  | N-CA-C | -10.71 | 97.83       | 112.94   |
| 9   | I     | 104  | LEU  | N-CA-C | -9.60  | 100.33      | 112.90   |
| 3   | C     | 258  | ILE  | N-CA-C | -9.01  | 104.06      | 111.81   |
| 1   | A     | 567  | LYS  | CA-C-N | -8.78  | 108.87      | 119.84   |
| 1   | A     | 567  | LYS  | C-N-CA | -8.78  | 108.87      | 119.84   |
| 6   | F     | 127  | GLU  | N-CA-C | -8.58  | 102.12      | 112.59   |
| 7   | G     | 62   | LEU  | CA-C-N | -8.52  | 109.19      | 119.84   |
| 7   | G     | 62   | LEU  | C-N-CA | -8.52  | 109.19      | 119.84   |
| 3   | C     | 39   | ALA  | N-CA-C | 8.41   | 123.67      | 113.41   |
| 4   | D     | 171  | GLY  | N-CA-C | -8.41  | 103.72      | 115.32   |
| 1   | A     | 1261 | LYS  | N-CA-C | -8.27  | 105.19      | 114.62   |
| 4   | D     | 7    | THR  | N-CA-C | 8.23   | 124.88      | 107.67   |
| 1   | A     | 320  | ARG  | CA-C-N | 7.99   | 129.82      | 119.84   |
| 1   | A     | 320  | ARG  | C-N-CA | 7.99   | 129.82      | 119.84   |
| 1   | A     | 582  | ILE  | CA-C-N | 7.95   | 127.88      | 119.85   |
| 1   | A     | 582  | ILE  | C-N-CA | 7.95   | 127.88      | 119.85   |
| 3   | C     | 38   | ILE  | N-CA-C | 7.81   | 117.92      | 110.42   |
| 1   | A     | 982  | THR  | N-CA-C | -7.71  | 99.63       | 110.50   |
| 1   | A     | 466  | SER  | N-CA-C | 7.68   | 122.40      | 112.26   |
| 1   | A     | 928  | LEU  | N-CA-C | -7.63  | 102.65      | 110.97   |
| 2   | B     | 395  | GLN  | N-CA-C | -7.63  | 100.46      | 110.53   |
| 1   | A     | 1262 | LYS  | N-CA-C | -7.60  | 103.00      | 111.82   |
| 7   | G     | 30   | LEU  | N-CA-C | -7.59  | 102.70      | 110.97   |
| 1   | A     | 1422 | ARG  | N-CA-C | -7.54  | 103.64      | 114.12   |
| 1   | A     | 564  | ALA  | N-CA-C | -7.53  | 103.01      | 111.14   |
| 1   | A     | 288  | ALA  | N-CA-C | -7.51  | 102.02      | 113.89   |
| 3   | C     | 40   | GLU  | N-CA-C | 7.48   | 121.72      | 112.59   |
| 8   | H     | 80   | ARG  | CA-C-N | 7.38   | 127.98      | 120.38   |
| 8   | H     | 80   | ARG  | C-N-CA | 7.38   | 127.98      | 120.38   |
| 2   | B     | 1020 | ARG  | N-CA-C | -7.38  | 103.32      | 111.36   |
| 2   | B     | 1052 | VAL  | N-CA-C | -7.36  | 103.68      | 110.82   |
| 1   | A     | 440  | ASP  | N-CA-C | -7.18  | 100.61      | 109.65   |
| 1   | A     | 729  | ALA  | N-CA-C | -7.16  | 103.56      | 111.36   |
| 1   | A     | 454  | SER  | N-CA-C | -7.16  | 104.42      | 113.01   |
| 7   | G     | 22   | MET  | N-CA-C | -7.15  | 103.17      | 112.68   |
| 6   | F     | 130  | ILE  | CA-C-N | 7.11   | 128.73      | 119.84   |
| 6   | F     | 130  | ILE  | C-N-CA | 7.11   | 128.73      | 119.84   |
| 1   | A     | 293  | GLU  | N-CA-C | -7.09  | 104.66      | 113.38   |
| 2   | B     | 681  | TRP  | N-CA-C | -7.04  | 100.78      | 111.56   |
| 1   | A     | 266  | LEU  | N-CA-C | -7.04  | 102.82      | 111.40   |
| 5   | E     | 171  | LYS  | N-CA-C | -7.01  | 99.55       | 110.42   |
| 4   | D     | 55   | ALA  | N-CA-C | -7.00  | 103.08      | 111.69   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 882  | THR  | N-CA-C  | 6.97  | 119.52      | 111.02   |
| 4   | D     | 72   | ARG  | N-CA-C  | -6.95 | 104.77      | 113.18   |
| 2   | B     | 296  | GLU  | N-CA-C  | -6.95 | 103.48      | 112.23   |
| 1   | A     | 950  | GLY  | N-CA-C  | -6.94 | 105.48      | 115.27   |
| 4   | D     | 38   | ILE  | N-CA-C  | 6.93  | 117.88      | 108.17   |
| 1   | A     | 539  | THR  | N-CA-C  | 6.93  | 119.41      | 108.67   |
| 1   | A     | 1403 | GLU  | N-CA-C  | 6.91  | 125.52      | 110.80   |
| 1   | A     | 291  | GLU  | N-CA-C  | -6.85 | 105.20      | 113.97   |
| 1   | A     | 425  | GLN  | N-CA-C  | -6.81 | 98.10       | 109.07   |
| 7   | G     | 129  | SER  | N-CA-C  | 6.81  | 118.14      | 108.74   |
| 1   | A     | 1291 | VAL  | CA-C-N  | 6.80  | 128.34      | 119.84   |
| 1   | A     | 1291 | VAL  | C-N-CA  | 6.80  | 128.34      | 119.84   |
| 4   | D     | 34   | GLN  | N-CA-C  | -6.76 | 101.81      | 110.19   |
| 1   | A     | 1311 | VAL  | N-CA-C  | 6.71  | 118.79      | 107.18   |
| 1   | A     | 738  | LYS  | N-CA-C  | 6.71  | 119.22      | 110.43   |
| 1   | A     | 472  | LEU  | N-CA-C  | 6.68  | 118.36      | 111.14   |
| 2   | B     | 208  | SER  | N-CA-C  | 6.67  | 119.91      | 110.50   |
| 9   | I     | 112  | SER  | N-CA-C  | -6.62 | 103.52      | 112.26   |
| 6   | F     | 77   | ASP  | N-CA-C  | -6.60 | 100.20      | 110.17   |
| 1   | A     | 30   | ILE  | N-CA-C  | 6.60  | 117.29      | 110.36   |
| 2   | B     | 66   | ASP  | N-CA-C  | -6.56 | 104.59      | 112.59   |
| 1   | A     | 453  | MET  | N-CA-C  | 6.54  | 120.72      | 112.87   |
| 2   | B     | 1173 | ALA  | N-CA-C  | 6.50  | 118.52      | 109.15   |
| 2   | B     | 872  | GLU  | N-CA-C  | -6.43 | 102.23      | 110.53   |
| 4   | D     | 173  | HIS  | CA-C-N  | 6.43  | 127.88      | 119.84   |
| 4   | D     | 173  | HIS  | C-N-CA  | 6.43  | 127.88      | 119.84   |
| 1   | A     | 337  | ARG  | N-CA-C  | 6.42  | 119.27      | 111.82   |
| 2   | B     | 292  | ILE  | N-CA-C  | 6.42  | 122.75      | 108.88   |
| 1   | A     | 227  | VAL  | N-CA-C  | 6.41  | 117.32      | 111.81   |
| 1   | A     | 158  | PRO  | N-CA-C  | -6.40 | 106.16      | 114.03   |
| 3   | C     | 165  | LYS  | N-CA-C  | -6.39 | 102.84      | 112.04   |
| 1   | A     | 1128 | ILE  | CB-CA-C | -6.38 | 106.28      | 111.71   |
| 2   | B     | 1009 | ASP  | N-CA-C  | -6.38 | 106.04      | 113.88   |
| 1   | A     | 360  | GLU  | N-CA-C  | -6.38 | 102.57      | 110.41   |
| 2   | B     | 363  | HIS  | N-CA-C  | -6.37 | 101.56      | 110.35   |
| 2   | B     | 535  | LEU  | N-CA-C  | -6.37 | 105.64      | 113.41   |
| 1   | A     | 1010 | ALA  | N-CA-C  | -6.37 | 104.39      | 111.71   |
| 1   | A     | 689  | LYS  | N-CA-C  | -6.29 | 104.86      | 112.54   |
| 1   | A     | 311  | GLN  | N-CA-C  | 6.26  | 123.65      | 109.81   |
| 5   | E     | 9    | ILE  | N-CA-C  | -6.25 | 105.73      | 111.67   |
| 1   | A     | 1413 | GLY  | N-CA-C  | -6.23 | 106.94      | 114.66   |
| 1   | A     | 242  | PRO  | CA-C-N  | 6.21  | 126.78      | 120.38   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 242  | PRO  | C-N-CA  | 6.21  | 126.78      | 120.38   |
| 4   | D     | 8    | PHE  | N-CA-C  | 6.20  | 124.00      | 110.80   |
| 1   | A     | 998  | LEU  | N-CA-C  | 6.17  | 119.58      | 109.76   |
| 1   | A     | 848  | ILE  | CA-C-N  | -6.13 | 110.66      | 121.70   |
| 1   | A     | 848  | ILE  | C-N-CA  | -6.13 | 110.66      | 121.70   |
| 1   | A     | 199  | LEU  | N-CA-C  | 6.09  | 118.22      | 108.41   |
| 1   | A     | 398  | GLU  | N-CA-C  | -6.09 | 102.92      | 110.41   |
| 5   | E     | 32   | GLN  | N-CA-C  | -6.07 | 105.36      | 112.89   |
| 1   | A     | 511  | ILE  | N-CA-C  | 6.07  | 117.54      | 110.62   |
| 12  | L     | 31   | CYS  | N-CA-C  | -6.06 | 100.87      | 109.96   |
| 9   | I     | 109  | ILE  | N-CA-C  | 6.04  | 115.05      | 106.53   |
| 7   | G     | 64   | THR  | N-CA-C  | -6.02 | 105.84      | 113.43   |
| 8   | H     | 4    | THR  | N-CA-C  | -6.02 | 100.20      | 109.52   |
| 1   | A     | 56   | PRO  | N-CA-C  | -5.99 | 100.13      | 112.47   |
| 2   | B     | 112  | LEU  | N-CA-C  | 5.99  | 119.34      | 110.48   |
| 2   | B     | 805  | THR  | N-CA-C  | 5.95  | 117.25      | 108.86   |
| 2   | B     | 555  | ILE  | N-CA-C  | -5.92 | 105.08      | 110.82   |
| 11  | K     | 8    | GLU  | N-CA-C  | -5.92 | 106.30      | 112.93   |
| 1   | A     | 424  | ILE  | N-CA-C  | 5.91  | 121.64      | 109.34   |
| 2   | B     | 1177 | HIS  | N-CA-C  | -5.90 | 106.33      | 112.93   |
| 10  | J     | 5    | VAL  | N-CA-C  | -5.89 | 101.98      | 109.58   |
| 9   | I     | 81   | ARG  | N-CA-C  | 5.87  | 118.39      | 110.88   |
| 1   | A     | 415  | LEU  | N-CA-C  | 5.87  | 119.26      | 111.75   |
| 2   | B     | 1045 | SER  | CA-C-N  | 5.84  | 127.15      | 119.84   |
| 2   | B     | 1045 | SER  | C-N-CA  | 5.84  | 127.15      | 119.84   |
| 9   | I     | 79   | HIS  | N-CA-C  | 5.84  | 119.71      | 112.47   |
| 1   | A     | 1021 | LEU  | N-CA-C  | -5.83 | 104.83      | 111.07   |
| 2   | B     | 428  | ILE  | N-CA-C  | -5.82 | 103.82      | 111.09   |
| 1   | A     | 1088 | VAL  | CB-CA-C | -5.81 | 108.18      | 113.70   |
| 2   | B     | 1163 | CYS  | N-CA-C  | -5.81 | 100.24      | 109.59   |
| 2   | B     | 1201 | LYS  | N-CA-C  | -5.80 | 103.95      | 111.02   |
| 4   | D     | 170  | THR  | N-CA-C  | 5.79  | 117.67      | 111.36   |
| 2   | B     | 1078 | GLY  | N-CA-C  | -5.79 | 107.00      | 115.63   |
| 2   | B     | 687  | GLU  | N-CA-C  | -5.79 | 104.88      | 112.41   |
| 5   | E     | 177  | ARG  | N-CA-C  | 5.76  | 119.07      | 110.14   |
| 2   | B     | 840  | ILE  | N-CA-C  | -5.75 | 99.46       | 107.80   |
| 9   | I     | 85   | PHE  | N-CA-C  | 5.74  | 118.92      | 110.59   |
| 1   | A     | 663  | SER  | N-CA-C  | 5.74  | 115.42      | 107.73   |
| 1   | A     | 562  | THR  | CA-C-N  | 5.74  | 127.01      | 119.84   |
| 1   | A     | 562  | THR  | C-N-CA  | 5.74  | 127.01      | 119.84   |
| 1   | A     | 683  | ILE  | N-CA-C  | -5.71 | 105.28      | 110.82   |
| 9   | I     | 105  | SER  | N-CA-C  | 5.70  | 120.00      | 112.25   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 1444 | MET  | N-CA-C  | 5.68  | 118.32      | 109.52   |
| 2   | B     | 934  | LYS  | N-CA-C  | 5.66  | 118.48      | 108.24   |
| 4   | D     | 176  | GLU  | N-CA-C  | -5.66 | 104.50      | 111.40   |
| 2   | B     | 1164 | GLY  | N-CA-C  | -5.65 | 107.92      | 115.32   |
| 2   | B     | 763  | GLN  | N-CA-C  | -5.65 | 101.68      | 110.10   |
| 1   | A     | 173  | THR  | N-CA-C  | -5.65 | 103.08      | 110.53   |
| 2   | B     | 1129 | ARG  | N-CA-C  | 5.64  | 119.44      | 109.96   |
| 3   | C     | 183  | TRP  | N-CA-C  | -5.64 | 98.01       | 107.99   |
| 1   | A     | 1445 | ILE  | CB-CA-C | -5.63 | 104.10      | 111.81   |
| 5   | E     | 65   | THR  | N-CA-C  | -5.62 | 102.16      | 110.48   |
| 1   | A     | 467  | THR  | N-CA-C  | 5.62  | 118.62      | 109.24   |
| 2   | B     | 558  | LEU  | N-CA-C  | 5.62  | 117.09      | 110.97   |
| 2   | B     | 1036 | ALA  | N-CA-C  | -5.61 | 105.56      | 112.90   |
| 8   | H     | 16   | ASP  | N-CA-C  | 5.60  | 119.39      | 107.91   |
| 7   | G     | 2    | PHE  | N-CA-C  | -5.58 | 102.63      | 110.50   |
| 6   | F     | 105  | ALA  | N-CA-C  | -5.57 | 102.03      | 110.39   |
| 2   | B     | 1139 | ILE  | N-CA-C  | -5.55 | 105.11      | 110.72   |
| 6   | F     | 120  | ILE  | N-CA-C  | -5.55 | 105.11      | 110.72   |
| 3   | C     | 96   | SER  | N-CA-C  | 5.52  | 117.47      | 109.07   |
| 2   | B     | 609  | ILE  | N-CA-C  | -5.52 | 99.80       | 107.80   |
| 1   | A     | 710  | LEU  | N-CA-C  | -5.49 | 105.39      | 111.71   |
| 2   | B     | 378  | LEU  | N-CA-C  | -5.48 | 105.21      | 112.34   |
| 11  | K     | 31   | VAL  | N-CA-C  | 5.46  | 116.58      | 108.65   |
| 1   | A     | 637  | LYS  | N-CA-C  | 5.45  | 117.30      | 111.36   |
| 2   | B     | 213  | ILE  | N-CA-C  | 5.45  | 117.15      | 108.87   |
| 1   | A     | 553  | VAL  | CA-C-N  | 5.43  | 125.10      | 119.56   |
| 1   | A     | 553  | VAL  | C-N-CA  | 5.43  | 125.10      | 119.56   |
| 1   | A     | 513  | SER  | CA-C-N  | 5.43  | 125.12      | 119.64   |
| 1   | A     | 513  | SER  | C-N-CA  | 5.43  | 125.12      | 119.64   |
| 8   | H     | 85   | GLY  | N-CA-C  | -5.39 | 108.42      | 114.40   |
| 8   | H     | 42   | ILE  | N-CA-C  | 5.39  | 115.46      | 108.35   |
| 1   | A     | 778  | GLY  | N-CA-C  | -5.38 | 105.89      | 112.77   |
| 2   | B     | 1213 | THR  | N-CA-C  | 5.37  | 117.20      | 109.04   |
| 1   | A     | 507  | VAL  | CB-CA-C | -5.36 | 108.61      | 113.70   |
| 7   | G     | 140  | LYS  | N-CA-C  | 5.36  | 119.44      | 113.01   |
| 8   | H     | 12   | VAL  | N-CA-C  | 5.35  | 115.30      | 108.12   |
| 2   | B     | 616  | ILE  | N-CA-C  | 5.33  | 115.80      | 108.12   |
| 5   | E     | 119  | SER  | N-CA-C  | -5.32 | 105.93      | 112.90   |
| 7   | G     | 114  | LEU  | N-CA-C  | -5.31 | 106.48      | 113.17   |
| 6   | F     | 153  | VAL  | N-CA-C  | 5.30  | 114.00      | 106.53   |
| 1   | A     | 1299 | VAL  | N-CA-C  | 5.30  | 117.69      | 108.95   |
| 9   | I     | 101  | PHE  | CA-C-N  | -5.29 | 115.84      | 123.03   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | I     | 101  | PHE  | C-N-CA  | -5.29 | 115.84      | 123.03   |
| 2   | B     | 1008 | PRO  | N-CA-C  | 5.28  | 119.00      | 111.13   |
| 7   | G     | 65   | ASP  | N-CA-C  | -5.28 | 102.35      | 109.95   |
| 1   | A     | 60   | SER  | N-CA-C  | 5.28  | 115.00      | 108.19   |
| 7   | G     | 40   | GLY  | N-CA-C  | -5.27 | 108.13      | 114.66   |
| 1   | A     | 999  | VAL  | N-CA-C  | -5.26 | 106.54      | 111.48   |
| 2   | B     | 650  | GLU  | N-CA-C  | 5.25  | 116.51      | 108.52   |
| 1   | A     | 55   | ASP  | N-CA-C  | 5.25  | 121.42      | 109.81   |
| 9   | I     | 119  | THR  | N-CA-C  | -5.25 | 107.26      | 113.97   |
| 2   | B     | 1066 | SER  | N-CA-C  | 5.24  | 119.30      | 113.01   |
| 1   | A     | 685  | GLU  | N-CA-C  | -5.24 | 105.75      | 111.82   |
| 6   | F     | 112  | GLU  | N-CA-C  | -5.23 | 106.16      | 113.37   |
| 2   | B     | 628  | THR  | N-CA-C  | -5.21 | 107.58      | 114.04   |
| 1   | A     | 1092 | LYS  | N-CA-C  | -5.20 | 105.50      | 111.07   |
| 1   | A     | 67   | CYS  | N-CA-C  | -5.20 | 99.73       | 110.80   |
| 1   | A     | 294  | SER  | N-CA-C  | -5.19 | 105.31      | 111.69   |
| 3   | C     | 91   | HIS  | N-CA-C  | 5.18  | 121.83      | 110.80   |
| 2   | B     | 99   | LYS  | CA-C-N  | 5.18  | 126.31      | 119.84   |
| 2   | B     | 99   | LYS  | C-N-CA  | 5.18  | 126.31      | 119.84   |
| 7   | G     | 127  | PRO  | CA-C-N  | 5.18  | 125.18      | 119.90   |
| 7   | G     | 127  | PRO  | C-N-CA  | 5.18  | 125.18      | 119.90   |
| 2   | B     | 424  | LEU  | N-CA-C  | -5.17 | 104.59      | 112.04   |
| 2   | B     | 1113 | VAL  | CB-CA-C | -5.16 | 106.35      | 111.30   |
| 2   | B     | 944  | THR  | N-CA-C  | 5.15  | 117.68      | 111.40   |
| 6   | F     | 108  | PHE  | N-CA-C  | 5.15  | 119.28      | 113.15   |
| 3   | C     | 193  | TYR  | N-CA-C  | 5.15  | 115.08      | 108.34   |
| 3   | C     | 235  | VAL  | N-CA-C  | -5.15 | 106.66      | 111.45   |
| 1   | A     | 990  | VAL  | N-CA-C  | -5.14 | 105.37      | 110.62   |
| 2   | B     | 277  | LYS  | N-CA-C  | 5.14  | 117.62      | 111.71   |
| 2   | B     | 825  | VAL  | N-CA-C  | 5.14  | 116.02      | 110.21   |
| 3   | C     | 148  | ARG  | N-CA-C  | 5.14  | 121.75      | 110.80   |
| 11  | K     | 19   | LEU  | N-CA-C  | 5.14  | 117.97      | 109.85   |
| 12  | L     | 34   | CYS  | N-CA-C  | -5.14 | 107.17      | 112.93   |
| 1   | A     | 229  | SER  | N-CA-C  | 5.13  | 115.79      | 107.32   |
| 7   | G     | 19   | GLY  | CA-C-N  | 5.13  | 126.25      | 119.84   |
| 7   | G     | 19   | GLY  | C-N-CA  | 5.13  | 126.25      | 119.84   |
| 1   | A     | 491  | VAL  | CA-C-N  | 5.13  | 126.25      | 119.84   |
| 1   | A     | 491  | VAL  | C-N-CA  | 5.13  | 126.25      | 119.84   |
| 2   | B     | 774  | GLY  | N-CA-C  | -5.13 | 108.71      | 114.40   |
| 2   | B     | 871  | THR  | N-CA-C  | 5.12  | 117.80      | 109.24   |
| 1   | A     | 1310 | GLY  | N-CA-C  | -5.12 | 102.06      | 110.56   |
| 2   | B     | 606  | LYS  | N-CA-C  | -5.12 | 107.70      | 114.04   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5   | E     | 55   | ARG  | N-CA-C  | 5.11  | 116.54      | 111.07   |
| 2   | B     | 964  | VAL  | N-CA-C  | 5.11  | 115.63      | 108.17   |
| 3   | C     | 225  | ALA  | N-CA-C  | 5.10  | 117.93      | 107.37   |
| 3   | C     | 70   | ILE  | CA-C-N  | 5.10  | 125.01      | 119.76   |
| 3   | C     | 70   | ILE  | C-N-CA  | 5.10  | 125.01      | 119.76   |
| 2   | B     | 693  | ILE  | N-CA-C  | 5.08  | 115.08      | 107.51   |
| 2   | B     | 526  | GLU  | N-CA-C  | 5.06  | 116.90      | 107.99   |
| 1   | A     | 931  | GLU  | N-CA-C  | -5.05 | 105.47      | 110.97   |
| 1   | A     | 1333 | ILE  | N-CA-C  | -5.04 | 105.07      | 110.36   |
| 2   | B     | 361  | LEU  | CA-C-N  | 5.04  | 126.14      | 119.84   |
| 2   | B     | 361  | LEU  | C-N-CA  | 5.04  | 126.14      | 119.84   |
| 2   | B     | 981  | ALA  | N-CA-C  | 5.04  | 116.18      | 108.52   |
| 1   | A     | 222  | LEU  | N-CA-C  | -5.04 | 102.31      | 110.32   |
| 1   | A     | 227  | VAL  | CB-CA-C | -5.04 | 105.76      | 111.55   |
| 1   | A     | 237  | THR  | N-CA-C  | -5.04 | 108.88      | 114.62   |
| 3   | C     | 38   | ILE  | CB-CA-C | -5.01 | 105.56      | 111.97   |
| 5   | E     | 6    | GLU  | N-CA-C  | -5.01 | 106.27      | 112.38   |
| 7   | G     | 145  | VAL  | N-CA-C  | 5.01  | 116.51      | 108.89   |
| 7   | G     | 45   | ILE  | N-CA-C  | -5.01 | 99.92       | 107.73   |
| 5   | E     | 52   | ARG  | CA-C-N  | 5.00  | 125.15      | 119.90   |
| 5   | E     | 52   | ARG  | C-N-CA  | 5.00  | 125.15      | 119.90   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 6964  | 0        | 3039     | 765     | 0            |
| 2   | B     | 5397  | 0        | 2399     | 488     | 0            |
| 3   | C     | 1317  | 0        | 590      | 66      | 0            |
| 4   | D     | 878   | 0        | 387      | 72      | 0            |
| 5   | E     | 1062  | 0        | 453      | 53      | 0            |
| 6   | F     | 417   | 0        | 180      | 126     | 0            |
| 7   | G     | 841   | 0        | 354      | 188     | 0            |
| 8   | H     | 659   | 0        | 296      | 31      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | I     | 587   | 0        | 235      | 33      | 0            |
| 10  | J     | 321   | 0        | 137      | 22      | 0            |
| 11  | K     | 565   | 0        | 260      | 13      | 0            |
| 12  | L     | 229   | 0        | 107      | 12      | 0            |
| All | All   | 19237 | 0        | 8437     | 1450    | 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 52.

All (1450) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 6:F:143:PHE:CB  | 7:G:68:ALA:CA    | 1.76                     | 1.61              |
| 1:A:344:ARG:CA  | 2:B:1129:ARG:HA  | 1.27                     | 1.60              |
| 6:F:143:PHE:CA  | 7:G:68:ALA:HB1   | 1.11                     | 1.58              |
| 2:B:1148:LYS:HA | 2:B:1200:ALA:CB  | 1.22                     | 1.57              |
| 1:A:1444:MET:CB | 7:G:10:ASN:CB    | 1.82                     | 1.57              |
| 2:B:312:GLU:CB  | 9:I:46:HIS:CB    | 1.83                     | 1.56              |
| 2:B:1148:LYS:CB | 2:B:1200:ALA:HB3 | 1.16                     | 1.55              |
| 2:B:1193:GLN:CB | 7:G:65:ASP:CB    | 1.84                     | 1.55              |
| 1:A:858:ASN:CB  | 1:A:1422:ARG:C   | 1.78                     | 1.53              |
| 2:B:1148:LYS:CA | 2:B:1200:ALA:HB3 | 1.02                     | 1.49              |
| 1:A:509:LEU:CB  | 1:A:1062:GLU:HA  | 1.03                     | 1.49              |
| 1:A:237:THR:CB  | 4:D:17:LYS:H     | 1.25                     | 1.48              |
| 1:A:89:PRO:CB   | 4:D:16:LYS:CB    | 1.88                     | 1.48              |
| 2:B:1148:LYS:CA | 2:B:1200:ALA:CB  | 1.79                     | 1.48              |
| 1:A:1444:MET:CB | 7:G:10:ASN:CA    | 1.89                     | 1.47              |
| 1:A:63:ARG:CB   | 1:A:411:ASP:HA   | 1.44                     | 1.46              |
| 2:B:1222:ARG:CB | 5:E:171:LYS:CA   | 1.94                     | 1.44              |
| 2:B:1193:GLN:CB | 7:G:65:ASP:CA    | 1.93                     | 1.43              |
| 6:F:73:ALA:N    | 7:G:70:PHE:H     | 0.96                     | 1.42              |
| 1:A:846:GLU:CB  | 2:B:1140:ALA:HB3 | 1.15                     | 1.41              |
| 2:B:1193:GLN:CB | 7:G:65:ASP:H     | 1.34                     | 1.40              |
| 1:A:509:LEU:CB  | 1:A:1062:GLU:CA  | 1.99                     | 1.40              |
| 1:A:636:GLU:CA  | 1:A:1056:SER:CB  | 1.84                     | 1.39              |
| 1:A:609:ASP:H   | 1:A:962:ARG:CB   | 1.35                     | 1.39              |
| 1:A:862:ASN:N   | 1:A:1420:ASP:CB  | 1.86                     | 1.39              |
| 1:A:1425:SER:C  | 2:B:1139:ILE:CB  | 1.96                     | 1.38              |
| 1:A:341:MET:O   | 2:B:1132:GLU:CA  | 1.70                     | 1.38              |
| 2:B:1145:SER:CB | 2:B:1195:HIS:C   | 1.98                     | 1.37              |
| 1:A:63:ARG:O    | 1:A:411:ASP:CB   | 1.71                     | 1.37              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:1193:GLN:CB  | 7:G:65:ASP:N     | 1.84                     | 1.37              |
| 6:F:73:ALA:N     | 7:G:70:PHE:N     | 1.72                     | 1.35              |
| 6:F:73:ALA:H     | 7:G:70:PHE:N     | 1.17                     | 1.35              |
| 1:A:566:ILE:CB   | 8:H:81:PRO:CB    | 2.05                     | 1.34              |
| 1:A:636:GLU:HA   | 1:A:1056:SER:CB  | 0.95                     | 1.34              |
| 1:A:858:ASN:CB   | 1:A:1422:ARG:CA  | 2.03                     | 1.34              |
| 1:A:846:GLU:CB   | 2:B:1140:ALA:CB  | 1.97                     | 1.33              |
| 1:A:129:LYS:CB   | 5:E:192:ARG:O    | 1.76                     | 1.33              |
| 1:A:453:MET:N    | 1:A:1066:VAL:CB  | 1.90                     | 1.33              |
| 2:B:1191:ILE:O   | 7:G:67:SER:CB    | 1.77                     | 1.33              |
| 1:A:609:ASP:N    | 1:A:962:ARG:CB   | 1.87                     | 1.32              |
| 1:A:859:SER:C    | 1:A:1421:CYS:CB  | 1.83                     | 1.32              |
| 2:B:1185:CYS:C   | 4:D:4:SER:N      | 1.88                     | 1.31              |
| 6:F:135:ARG:N    | 7:G:15:PRO:CB    | 1.93                     | 1.31              |
| 1:A:766:GLY:HA3  | 1:A:820:GLY:N    | 1.46                     | 1.30              |
| 1:A:1429:ILE:C   | 2:B:1147:LEU:CB  | 2.04                     | 1.30              |
| 6:F:142:SER:HA   | 7:G:69:GLU:C     | 1.57                     | 1.30              |
| 1:A:1430:LEU:C   | 2:B:1143:ALA:O   | 1.74                     | 1.29              |
| 6:F:142:SER:HA   | 7:G:69:GLU:O     | 1.19                     | 1.28              |
| 6:F:138:LEU:CB   | 7:G:59:GLY:O     | 1.81                     | 1.28              |
| 1:A:859:SER:O    | 1:A:1421:CYS:CB  | 1.80                     | 1.28              |
| 1:A:1427:ASN:CB  | 2:B:1142:GLY:H   | 1.47                     | 1.26              |
| 1:A:1444:MET:CB  | 7:G:10:ASN:C     | 2.06                     | 1.26              |
| 2:B:1149:GLU:C   | 2:B:1156:ASP:CB  | 2.08                     | 1.26              |
| 1:A:846:GLU:CB   | 2:B:1137:CYS:HA  | 1.62                     | 1.25              |
| 1:A:766:GLY:O    | 1:A:817:ALA:C    | 1.77                     | 1.25              |
| 1:A:630:ILE:O    | 1:A:876:ALA:CA   | 1.83                     | 1.24              |
| 2:B:1223:ASP:HA  | 5:E:168:TYR:CB   | 1.67                     | 1.23              |
| 6:F:72:LYS:N     | 7:G:69:GLU:C     | 1.96                     | 1.23              |
| 1:A:846:GLU:N    | 2:B:1140:ALA:CB  | 1.93                     | 1.23              |
| 1:A:1425:SER:O   | 2:B:1139:ILE:CB  | 1.87                     | 1.22              |
| 2:B:1148:LYS:CB  | 2:B:1200:ALA:CB  | 2.03                     | 1.22              |
| 6:F:143:PHE:CA   | 7:G:68:ALA:CB    | 1.79                     | 1.21              |
| 1:A:386:ASP:CB   | 6:F:104:ASN:O    | 1.89                     | 1.21              |
| 1:A:503:GLN:O    | 1:A:1061:GLY:HA2 | 1.35                     | 1.20              |
| 6:F:142:SER:CA   | 7:G:69:GLU:O     | 1.87                     | 1.20              |
| 6:F:72:LYS:N     | 7:G:70:PHE:N     | 1.88                     | 1.20              |
| 1:A:452:LYS:CA   | 1:A:846:GLU:HA   | 1.70                     | 1.19              |
| 1:A:515:GLN:CB   | 1:A:1069:ALA:HA  | 1.72                     | 1.19              |
| 1:A:635:ARG:N    | 1:A:877:HIS:H    | 1.40                     | 1.19              |
| 1:A:1431:GLY:HA3 | 2:B:1147:LEU:N   | 1.55                     | 1.19              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1444:MET:CB | 6:F:72:LYS:HA    | 1.66                     | 1.19              |
| 1:A:341:MET:HA  | 2:B:1135:ARG:CB  | 1.73                     | 1.18              |
| 1:A:344:ARG:C   | 2:B:1129:ARG:HA  | 1.67                     | 1.18              |
| 1:A:858:ASN:CB  | 1:A:1422:ARG:O   | 1.90                     | 1.18              |
| 1:A:341:MET:O   | 2:B:1132:GLU:HA  | 1.23                     | 1.18              |
| 2:B:1145:SER:CB | 2:B:1195:HIS:O   | 1.91                     | 1.18              |
| 1:A:518:LYS:CB  | 1:A:1364:ASN:N   | 2.07                     | 1.18              |
| 1:A:1431:GLY:C  | 2:B:1143:ALA:O   | 1.87                     | 1.18              |
| 1:A:810:PRO:CB  | 2:B:731:VAL:N    | 2.07                     | 1.17              |
| 2:B:1192:TYR:HA | 7:G:67:SER:CB    | 1.73                     | 1.17              |
| 1:A:344:ARG:CA  | 2:B:1129:ARG:CA  | 2.23                     | 1.17              |
| 1:A:1444:MET:CB | 2:B:1165:ILE:N   | 2.07                     | 1.17              |
| 2:B:1148:LYS:O  | 2:B:1198:TYR:C   | 1.81                     | 1.17              |
| 1:A:63:ARG:O    | 1:A:411:ASP:CA   | 1.85                     | 1.16              |
| 1:A:858:ASN:CB  | 1:A:1422:ARG:HA  | 1.72                     | 1.16              |
| 1:A:766:GLY:CA  | 1:A:820:GLY:H    | 1.57                     | 1.16              |
| 1:A:810:PRO:CB  | 2:B:731:VAL:HA   | 1.74                     | 1.15              |
| 1:A:630:ILE:O   | 1:A:876:ALA:HA   | 0.98                     | 1.15              |
| 1:A:237:THR:CB  | 4:D:17:LYS:N     | 2.08                     | 1.15              |
| 2:B:1148:LYS:HA | 2:B:1200:ALA:HB2 | 1.25                     | 1.15              |
| 2:B:1192:TYR:CB | 7:G:62:LEU:CB    | 2.23                     | 1.15              |
| 1:A:341:MET:O   | 2:B:1132:GLU:C   | 1.90                     | 1.14              |
| 1:A:810:PRO:CB  | 2:B:731:VAL:CA   | 2.25                     | 1.14              |
| 2:B:1185:CYS:CA | 4:D:4:SER:N      | 2.11                     | 1.14              |
| 2:B:1219:ASP:CB | 7:G:59:GLY:C     | 2.20                     | 1.14              |
| 1:A:383:TYR:O   | 6:F:105:ALA:HB1  | 1.46                     | 1.14              |
| 1:A:1427:ASN:CB | 2:B:1142:GLY:N   | 2.10                     | 1.14              |
| 1:A:443:LEU:H   | 2:B:1153:GLU:CB  | 1.60                     | 1.14              |
| 1:A:846:GLU:N   | 2:B:1140:ALA:HB1 | 1.39                     | 1.14              |
| 1:A:77:CYS:O    | 1:A:78:PRO:O     | 1.65                     | 1.13              |
| 1:A:845:LEU:C   | 2:B:1140:ALA:HB1 | 1.73                     | 1.13              |
| 1:A:862:ASN:CB  | 1:A:1422:ARG:CB  | 2.27                     | 1.13              |
| 1:A:490:HIS:O   | 2:B:1153:GLU:CB  | 1.84                     | 1.12              |
| 6:F:135:ARG:CB  | 7:G:66:GLY:O     | 1.96                     | 1.12              |
| 1:A:846:GLU:CB  | 2:B:1137:CYS:CA  | 2.27                     | 1.12              |
| 1:A:846:GLU:CB  | 2:B:1137:CYS:O   | 1.98                     | 1.12              |
| 1:A:1444:MET:CB | 2:B:1164:GLY:C   | 2.21                     | 1.12              |
| 2:B:1193:GLN:CB | 7:G:65:ASP:C     | 2.22                     | 1.12              |
| 1:A:11:LEU:HA   | 7:G:65:ASP:O     | 1.48                     | 1.11              |
| 1:A:1431:GLY:N  | 2:B:1143:ALA:O   | 1.83                     | 1.11              |
| 1:A:10:PRO:CB   | 7:G:67:SER:HA    | 1.80                     | 1.11              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:B:1149:GLU:CB | 2:B:1158:PHE:N  | 2.12                     | 1.11              |
| 1:A:858:ASN:N   | 1:A:1422:ARG:HA | 1.64                     | 1.11              |
| 1:A:1452:LYS:CB | 7:G:28:THR:CB   | 2.29                     | 1.11              |
| 1:A:344:ARG:C   | 2:B:1129:ARG:CA | 2.21                     | 1.11              |
| 1:A:518:LYS:CB  | 1:A:1364:ASN:H  | 1.64                     | 1.10              |
| 1:A:513:SER:O   | 1:A:1367:HIS:CB | 1.99                     | 1.10              |
| 1:A:450:LEU:O   | 1:A:842:VAL:N   | 1.68                     | 1.09              |
| 1:A:767:GLN:HA  | 1:A:818:MET:CB  | 1.79                     | 1.09              |
| 1:A:858:ASN:CA  | 1:A:1422:ARG:HA | 1.81                     | 1.09              |
| 1:A:1431:GLY:N  | 2:B:1147:LEU:CB | 2.15                     | 1.09              |
| 2:B:1193:GLN:N  | 7:G:62:LEU:CB   | 2.15                     | 1.09              |
| 1:A:1430:LEU:C  | 2:B:1147:LEU:H  | 1.60                     | 1.09              |
| 2:B:1219:ASP:HA | 6:F:138:LEU:C   | 1.77                     | 1.09              |
| 1:A:344:ARG:HA  | 2:B:1129:ARG:CA | 1.80                     | 1.09              |
| 1:A:1428:VAL:HA | 2:B:1138:MET:CB | 1.84                     | 1.08              |
| 1:A:777:PHE:O   | 2:B:400:HIS:CB  | 1.97                     | 1.08              |
| 1:A:450:LEU:C   | 1:A:843:LYS:H   | 1.61                     | 1.08              |
| 1:A:452:LYS:HA  | 1:A:846:GLU:CA  | 1.84                     | 1.07              |
| 2:B:1146:PHE:C  | 2:B:1197:PRO:N  | 2.11                     | 1.07              |
| 1:A:11:LEU:CB   | 7:G:65:ASP:C    | 2.19                     | 1.06              |
| 1:A:635:ARG:HA  | 1:A:874:ASP:N   | 1.42                     | 1.06              |
| 2:B:401:PHE:C   | 2:B:517:THR:H   | 1.54                     | 1.06              |
| 1:A:383:TYR:O   | 6:F:105:ALA:CB  | 2.04                     | 1.05              |
| 1:A:450:LEU:C   | 1:A:843:LYS:N   | 2.11                     | 1.05              |
| 1:A:766:GLY:CA  | 1:A:820:GLY:N   | 2.17                     | 1.05              |
| 1:A:1393:ASN:HA | 1:A:1399:ARG:H  | 1.18                     | 1.05              |
| 1:A:510:GLN:O   | 1:A:1067:LEU:CB | 2.04                     | 1.05              |
| 1:A:1448:GLU:CB | 7:G:27:LYS:O    | 2.05                     | 1.05              |
| 1:A:452:LYS:CB  | 1:A:1066:VAL:CB | 2.34                     | 1.04              |
| 1:A:858:ASN:H   | 1:A:1422:ARG:HA | 1.20                     | 1.04              |
| 1:A:862:ASN:CA  | 1:A:1420:ASP:CB | 2.34                     | 1.04              |
| 1:A:1431:GLY:CA | 2:B:1147:LEU:N  | 2.20                     | 1.04              |
| 2:B:1223:ASP:CA | 5:E:168:TYR:CB  | 2.35                     | 1.03              |
| 1:A:341:MET:C   | 2:B:1132:GLU:HA | 1.82                     | 1.03              |
| 1:A:608:ILE:CA  | 1:A:962:ARG:CB  | 2.36                     | 1.03              |
| 1:A:1444:MET:CB | 7:G:10:ASN:HA   | 1.86                     | 1.03              |
| 2:B:1219:ASP:CB | 7:G:58:ARG:C    | 2.31                     | 1.03              |
| 1:A:503:GLN:O   | 1:A:1061:GLY:CA | 2.05                     | 1.02              |
| 2:B:1146:PHE:N  | 2:B:1195:HIS:O  | 1.92                     | 1.02              |
| 1:A:810:PRO:HA  | 2:B:729:ILE:O   | 1.60                     | 1.02              |
| 1:A:1427:ASN:CB | 2:B:1142:GLY:CA | 2.35                     | 1.02              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 6:F:72:LYS:C    | 7:G:70:PHE:H     | 1.52                     | 1.02              |
| 1:A:23:SER:HA   | 4:D:13:ARG:CB    | 1.90                     | 1.02              |
| 1:A:518:LYS:H   | 1:A:1367:HIS:CB  | 1.72                     | 1.02              |
| 1:A:504:LEU:HA  | 1:A:1061:GLY:O   | 1.59                     | 1.02              |
| 1:A:1427:ASN:CB | 2:B:1142:GLY:HA2 | 1.89                     | 1.02              |
| 1:A:452:LYS:HA  | 1:A:846:GLU:HA   | 1.02                     | 1.01              |
| 1:A:452:LYS:CB  | 1:A:1066:VAL:CA  | 2.38                     | 1.01              |
| 2:B:1192:TYR:C  | 7:G:62:LEU:CB    | 2.34                     | 1.01              |
| 9:I:3:THR:O     | 9:I:43:VAL:N     | 1.88                     | 1.01              |
| 1:A:514:PRO:CB  | 1:A:1370:LEU:CB  | 2.39                     | 1.01              |
| 1:A:1431:GLY:CA | 2:B:1143:ALA:O   | 2.09                     | 1.00              |
| 1:A:452:LYS:CB  | 1:A:1066:VAL:N   | 2.25                     | 1.00              |
| 1:A:515:GLN:CB  | 1:A:1069:ALA:CA  | 2.38                     | 1.00              |
| 1:A:1430:LEU:C  | 2:B:1147:LEU:CB  | 2.34                     | 1.00              |
| 1:A:1430:LEU:N  | 2:B:1147:LEU:CB  | 2.24                     | 1.00              |
| 6:F:138:LEU:H   | 7:G:60:ARG:HA    | 1.26                     | 1.00              |
| 6:F:75:PRO:HA   | 7:G:26:LEU:H     | 1.23                     | 0.99              |
| 6:F:143:PHE:N   | 7:G:68:ALA:HB1   | 1.76                     | 0.99              |
| 1:A:516:SER:N   | 1:A:1367:HIS:C   | 2.16                     | 0.99              |
| 6:F:77:ASP:N    | 7:G:23:LYS:N     | 1.99                     | 0.99              |
| 1:A:766:GLY:O   | 1:A:815:PHE:O    | 1.78                     | 0.99              |
| 1:A:341:MET:O   | 2:B:1132:GLU:O   | 1.78                     | 0.99              |
| 2:B:1148:LYS:HA | 2:B:1200:ALA:CA  | 1.93                     | 0.98              |
| 1:A:492:PRO:HA  | 2:B:1157:ALA:HB1 | 1.45                     | 0.98              |
| 6:F:133:VAL:O   | 7:G:15:PRO:CB    | 2.12                     | 0.98              |
| 1:A:63:ARG:CB   | 1:A:411:ASP:CA   | 2.41                     | 0.98              |
| 2:B:1148:LYS:O  | 2:B:1199:ALA:N   | 1.96                     | 0.97              |
| 1:A:863:VAL:CB  | 2:B:1224:PHE:C   | 2.37                     | 0.97              |
| 1:A:10:PRO:CB   | 7:G:67:SER:CA    | 2.41                     | 0.96              |
| 1:A:341:MET:CA  | 2:B:1135:ARG:CB  | 2.42                     | 0.96              |
| 1:A:608:ILE:C   | 1:A:962:ARG:CB   | 2.38                     | 0.96              |
| 6:F:77:ASP:H    | 7:G:24:GLN:H     | 1.07                     | 0.96              |
| 1:A:859:SER:C   | 1:A:1437:GLY:N   | 2.23                     | 0.96              |
| 1:A:344:ARG:HA  | 2:B:1129:ARG:HA  | 0.99                     | 0.96              |
| 1:A:766:GLY:O   | 1:A:816:HIS:C    | 2.02                     | 0.96              |
| 2:B:1219:ASP:CB | 6:F:138:LEU:CB   | 2.43                     | 0.96              |
| 6:F:135:ARG:H   | 7:G:15:PRO:CB    | 1.77                     | 0.96              |
| 1:A:453:MET:H   | 1:A:1066:VAL:CB  | 1.64                     | 0.96              |
| 1:A:1429:ILE:O  | 2:B:1147:LEU:CB  | 2.12                     | 0.96              |
| 2:B:1193:GLN:O  | 7:G:65:ASP:O     | 1.84                     | 0.95              |
| 3:C:39:ALA:HA   | 3:C:164:ALA:HB3  | 1.47                     | 0.95              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:862:ASN:H    | 1:A:1420:ASP:CB | 1.75                     | 0.95              |
| 6:F:145:ASP:CB   | 7:G:17:PHE:C    | 2.30                     | 0.94              |
| 1:A:1448:GLU:HA  | 7:G:32:GLU:H    | 1.31                     | 0.94              |
| 1:A:518:LYS:N    | 1:A:1367:HIS:CB | 2.28                     | 0.94              |
| 1:A:55:ASP:C     | 1:A:57:ARG:H    | 1.72                     | 0.94              |
| 1:A:235:ILE:C    | 4:D:16:LYS:H    | 1.76                     | 0.94              |
| 2:B:1223:ASP:CB  | 5:E:168:TYR:CB  | 2.45                     | 0.94              |
| 1:A:1432:GLN:O   | 2:B:1138:MET:O  | 1.86                     | 0.93              |
| 3:C:47:ASP:HA    | 12:L:69:ALA:HB3 | 1.50                     | 0.93              |
| 2:B:1149:GLU:O   | 2:B:1156:ASP:CB | 2.17                     | 0.93              |
| 1:A:387:ARG:N    | 6:F:104:ASN:CB  | 2.32                     | 0.93              |
| 1:A:846:GLU:CB   | 2:B:1137:CYS:C  | 2.41                     | 0.93              |
| 1:A:1444:MET:CB  | 7:G:11:ILE:N    | 2.31                     | 0.92              |
| 2:B:1192:TYR:CB  | 7:G:67:SER:O    | 2.17                     | 0.92              |
| 6:F:77:ASP:H     | 7:G:23:LYS:N    | 1.67                     | 0.92              |
| 1:A:640:GLN:CB   | 6:F:87:LYS:CB   | 2.47                     | 0.92              |
| 1:A:608:ILE:HA   | 1:A:962:ARG:CB  | 1.99                     | 0.92              |
| 1:A:1432:GLN:O   | 2:B:1141:HIS:CB | 2.11                     | 0.92              |
| 6:F:72:LYS:N     | 7:G:69:GLU:CA   | 2.28                     | 0.92              |
| 1:A:635:ARG:CA   | 1:A:874:ASP:N   | 2.30                     | 0.92              |
| 1:A:766:GLY:C    | 1:A:815:PHE:O   | 2.12                     | 0.92              |
| 1:A:1444:MET:CB  | 6:F:72:LYS:CA   | 2.47                     | 0.91              |
| 1:A:800:VAL:HA   | 1:A:814:PHE:HA  | 1.51                     | 0.91              |
| 1:A:452:LYS:CB   | 1:A:846:GLU:HA  | 1.99                     | 0.91              |
| 1:A:11:LEU:CA    | 7:G:65:ASP:O    | 2.09                     | 0.91              |
| 1:A:1431:GLY:HA3 | 2:B:1147:LEU:H  | 1.36                     | 0.91              |
| 1:A:1430:LEU:O   | 2:B:1143:ALA:O  | 1.89                     | 0.91              |
| 1:A:1427:ASN:C   | 2:B:1138:MET:O  | 2.14                     | 0.90              |
| 1:A:1446:ASP:O   | 7:G:29:LYS:CB   | 2.19                     | 0.90              |
| 1:A:1431:GLY:CA  | 2:B:1147:LEU:H  | 1.82                     | 0.90              |
| 1:A:800:VAL:HA   | 1:A:814:PHE:CA  | 1.99                     | 0.90              |
| 1:A:1442:ASP:HA  | 2:B:1216:LEU:O  | 1.72                     | 0.90              |
| 1:A:11:LEU:CB    | 7:G:65:ASP:O    | 2.20                     | 0.89              |
| 1:A:767:GLN:CA   | 1:A:818:MET:CB  | 2.44                     | 0.89              |
| 8:H:4:THR:HA     | 8:H:60:ALA:HB2  | 1.52                     | 0.89              |
| 6:F:138:LEU:N    | 7:G:60:ARG:HA   | 1.79                     | 0.89              |
| 6:F:134:ILE:C    | 7:G:15:PRO:CB   | 2.45                     | 0.89              |
| 2:B:1149:GLU:CB  | 2:B:1157:ALA:C  | 2.46                     | 0.88              |
| 1:A:1427:ASN:N   | 2:B:1139:ILE:CA | 2.30                     | 0.88              |
| 1:A:496:GLU:C    | 7:G:63:PRO:O    | 2.16                     | 0.88              |
| 1:A:1425:SER:CA  | 2:B:1139:ILE:CB | 2.52                     | 0.88              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 6:F:77:ASP:H     | 7:G:24:GLN:N    | 1.71                     | 0.88              |
| 1:A:1065:GLY:HA3 | 1:A:1435:PRO:C  | 1.99                     | 0.88              |
| 1:A:515:GLN:CB   | 1:A:1069:ALA:N  | 2.37                     | 0.88              |
| 1:A:1444:MET:O   | 6:F:72:LYS:C    | 2.16                     | 0.87              |
| 1:A:845:LEU:O    | 1:A:1435:PRO:C  | 2.17                     | 0.87              |
| 1:A:766:GLY:HA3  | 1:A:819:GLY:C   | 1.94                     | 0.87              |
| 1:A:1428:VAL:HA  | 2:B:1138:MET:CA | 1.95                     | 0.87              |
| 2:B:1146:PHE:O   | 2:B:1197:PRO:N  | 2.06                     | 0.87              |
| 1:A:635:ARG:HA   | 1:A:874:ASP:H   | 1.41                     | 0.86              |
| 1:A:1431:GLY:HA3 | 2:B:1146:PHE:C  | 2.01                     | 0.86              |
| 1:A:235:ILE:O    | 4:D:16:LYS:N    | 2.09                     | 0.86              |
| 2:B:168:GLY:H    | 2:B:450:ALA:HB1 | 1.39                     | 0.86              |
| 1:A:859:SER:O    | 1:A:1437:GLY:N  | 2.09                     | 0.86              |
| 1:A:1452:LYS:H   | 7:G:28:THR:CB   | 1.88                     | 0.86              |
| 1:A:625:SER:HA   | 1:A:1362:TYR:O  | 1.75                     | 0.85              |
| 1:A:1431:GLY:N   | 2:B:1147:LEU:H  | 1.75                     | 0.85              |
| 2:B:401:PHE:C    | 2:B:517:THR:N   | 2.34                     | 0.85              |
| 6:F:77:ASP:N     | 7:G:24:GLN:H    | 1.74                     | 0.85              |
| 2:B:1145:SER:CB  | 2:B:1196:ILE:N  | 2.34                     | 0.85              |
| 3:C:164:ALA:HA   | 3:C:167:HIS:O   | 1.76                     | 0.85              |
| 1:A:859:SER:CB   | 1:A:1426:GLU:CB | 2.55                     | 0.85              |
| 1:A:799:PHE:HA   | 1:A:818:MET:CB  | 2.06                     | 0.84              |
| 1:A:847:ASP:O    | 2:B:1141:HIS:C  | 2.20                     | 0.84              |
| 1:A:1443:VAL:HA  | 7:G:69:GLU:O    | 1.76                     | 0.84              |
| 1:A:492:PRO:HA   | 2:B:1157:ALA:CB | 2.08                     | 0.84              |
| 3:C:47:ASP:HA    | 12:L:69:ALA:CB  | 2.06                     | 0.84              |
| 1:A:443:LEU:N    | 2:B:1153:GLU:CB | 2.41                     | 0.84              |
| 1:A:341:MET:C    | 2:B:1135:ARG:CB | 2.51                     | 0.84              |
| 6:F:75:PRO:N     | 7:G:26:LEU:CB   | 2.41                     | 0.84              |
| 1:A:634:THR:O    | 1:A:874:ASP:CB  | 2.26                     | 0.83              |
| 2:B:1146:PHE:N   | 2:B:1195:HIS:C  | 2.35                     | 0.83              |
| 1:A:1393:ASN:HA  | 1:A:1399:ARG:N  | 1.92                     | 0.83              |
| 1:A:1427:ASN:CB  | 2:B:1138:MET:O  | 2.27                     | 0.83              |
| 1:A:810:PRO:CB   | 2:B:730:ARG:C   | 2.52                     | 0.83              |
| 2:B:1146:PHE:O   | 2:B:1197:PRO:CA | 2.26                     | 0.83              |
| 1:A:1430:LEU:C   | 2:B:1147:LEU:N  | 2.37                     | 0.83              |
| 1:A:1430:LEU:CA  | 2:B:1147:LEU:CB | 2.56                     | 0.83              |
| 2:B:1193:GLN:CA  | 7:G:65:ASP:H    | 1.92                     | 0.82              |
| 2:B:1219:ASP:CB  | 7:G:58:ARG:O    | 2.27                     | 0.82              |
| 1:A:123:ARG:CB   | 5:E:128:PRO:CB  | 2.56                     | 0.82              |
| 2:B:1145:SER:CB  | 7:G:63:PRO:CB   | 2.58                     | 0.82              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:514:PRO:HA  | 1:A:1367:HIS:HA | 1.62                     | 0.82              |
| 6:F:138:LEU:H   | 7:G:60:ARG:CA   | 1.91                     | 0.82              |
| 1:A:635:ARG:N   | 1:A:877:HIS:N   | 2.25                     | 0.82              |
| 2:B:1219:ASP:HA | 6:F:138:LEU:CB  | 2.09                     | 0.82              |
| 1:A:800:VAL:N   | 1:A:815:PHE:C   | 2.37                     | 0.82              |
| 2:B:1219:ASP:CB | 7:G:59:GLY:O    | 2.28                     | 0.82              |
| 1:A:626:ASN:H   | 1:A:1362:TYR:C  | 1.87                     | 0.81              |
| 2:B:1149:GLU:O  | 2:B:1198:TYR:CB | 2.26                     | 0.81              |
| 1:A:630:ILE:C   | 1:A:876:ALA:HA  | 2.01                     | 0.81              |
| 2:B:1185:CYS:HA | 4:D:4:SER:N     | 1.94                     | 0.81              |
| 2:B:1148:LYS:N  | 2:B:1197:PRO:N  | 2.20                     | 0.81              |
| 2:B:1192:TYR:CA | 7:G:67:SER:CB   | 2.58                     | 0.81              |
| 2:B:312:GLU:H   | 9:I:46:HIS:HA   | 1.45                     | 0.81              |
| 6:F:72:LYS:C    | 7:G:11:ILE:O    | 2.21                     | 0.81              |
| 1:A:534:LEU:O   | 1:A:574:GLY:HA3 | 1.81                     | 0.80              |
| 1:A:766:GLY:O   | 1:A:818:MET:N   | 2.13                     | 0.80              |
| 4:D:130:LEU:C   | 4:D:132:GLN:H   | 1.86                     | 0.80              |
| 1:A:633:VAL:C   | 1:A:877:HIS:CA  | 2.46                     | 0.80              |
| 6:F:73:ALA:N    | 7:G:70:PHE:CA   | 2.45                     | 0.80              |
| 1:A:71:GLN:CB   | 1:A:408:ASP:CB  | 2.59                     | 0.80              |
| 6:F:78:GLN:CB   | 7:G:23:LYS:CB   | 2.60                     | 0.80              |
| 1:A:634:THR:C   | 1:A:877:HIS:H   | 1.87                     | 0.80              |
| 1:A:800:VAL:HA  | 1:A:814:PHE:O   | 1.81                     | 0.80              |
| 6:F:146:TRP:CB  | 7:G:18:PHE:O    | 2.29                     | 0.80              |
| 2:B:1223:ASP:O  | 5:E:170:LEU:CB  | 2.29                     | 0.80              |
| 6:F:142:SER:N   | 7:G:69:GLU:O    | 2.14                     | 0.79              |
| 1:A:235:ILE:C   | 4:D:16:LYS:N    | 2.39                     | 0.79              |
| 1:A:634:THR:C   | 1:A:874:ASP:CB  | 2.56                     | 0.79              |
| 1:A:1432:GLN:N  | 2:B:1143:ALA:O  | 2.05                     | 0.79              |
| 6:F:111:LEU:C   | 6:F:113:GLY:H   | 1.90                     | 0.79              |
| 1:A:766:GLY:O   | 1:A:817:ALA:N   | 2.16                     | 0.78              |
| 2:B:1145:SER:CA | 2:B:1195:HIS:O  | 2.30                     | 0.78              |
| 1:A:63:ARG:CA   | 1:A:411:ASP:HA  | 2.01                     | 0.78              |
| 1:A:452:LYS:CB  | 1:A:1066:VAL:H  | 1.94                     | 0.78              |
| 1:A:386:ASP:C   | 6:F:104:ASN:CB  | 2.56                     | 0.78              |
| 1:A:767:GLN:O   | 1:A:819:GLY:HA2 | 1.83                     | 0.78              |
| 6:F:146:TRP:CA  | 7:G:18:PHE:O    | 2.24                     | 0.78              |
| 1:A:55:ASP:C    | 1:A:57:ARG:N    | 2.41                     | 0.77              |
| 1:A:10:PRO:N    | 7:G:67:SER:CA   | 2.37                     | 0.77              |
| 2:B:1219:ASP:HA | 6:F:139:PRO:N   | 1.99                     | 0.77              |
| 1:A:2:VAL:O     | 1:A:494:SER:C   | 2.17                     | 0.77              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:453:MET:CA  | 1:A:1066:VAL:CB  | 2.63                     | 0.77              |
| 1:A:520:CYS:CB  | 1:A:1071:SER:N   | 2.47                     | 0.77              |
| 1:A:635:ARG:H   | 1:A:877:HIS:H    | 1.31                     | 0.77              |
| 1:A:588:LEU:O   | 1:A:606:LEU:HA   | 1.85                     | 0.77              |
| 2:B:401:PHE:O   | 2:B:517:THR:CB   | 2.33                     | 0.76              |
| 2:B:1192:TYR:HA | 7:G:67:SER:C     | 2.10                     | 0.76              |
| 1:A:452:LYS:C   | 1:A:1066:VAL:CB  | 2.58                     | 0.76              |
| 2:B:1148:LYS:HA | 2:B:1200:ALA:N   | 2.00                     | 0.76              |
| 2:B:1149:GLU:CB | 2:B:1158:PHE:H   | 1.95                     | 0.76              |
| 1:A:16:GLU:O    | 1:A:1441:PHE:N   | 2.11                     | 0.76              |
| 2:B:392:ARG:CA  | 9:I:90:GLN:CB    | 2.64                     | 0.76              |
| 1:A:516:SER:N   | 1:A:1367:HIS:O   | 2.19                     | 0.75              |
| 2:B:1159:ARG:CB | 7:G:64:THR:CB    | 2.64                     | 0.75              |
| 1:A:1393:ASN:HA | 1:A:1396:ALA:O   | 1.86                     | 0.75              |
| 1:A:846:GLU:N   | 2:B:1140:ALA:HB2 | 2.01                     | 0.75              |
| 2:B:1219:ASP:CA | 6:F:138:LEU:CB   | 2.65                     | 0.75              |
| 2:B:1222:ARG:CB | 5:E:171:LYS:C    | 2.60                     | 0.75              |
| 1:A:810:PRO:CA  | 2:B:729:ILE:O    | 2.33                     | 0.75              |
| 2:B:1194:ILE:O  | 7:G:64:THR:CA    | 2.35                     | 0.74              |
| 1:A:1449:SER:HA | 7:G:28:THR:N     | 2.00                     | 0.74              |
| 2:B:392:ARG:CB  | 9:I:90:GLN:CB    | 2.65                     | 0.74              |
| 6:F:73:ALA:N    | 7:G:11:ILE:O     | 2.20                     | 0.74              |
| 6:F:133:VAL:C   | 7:G:15:PRO:CB    | 2.60                     | 0.74              |
| 1:A:10:PRO:CB   | 7:G:66:GLY:O     | 2.36                     | 0.74              |
| 2:B:392:ARG:C   | 9:I:90:GLN:CB    | 2.51                     | 0.74              |
| 1:A:1444:MET:CB | 2:B:1165:ILE:CA  | 2.66                     | 0.74              |
| 2:B:1193:GLN:CB | 7:G:65:ASP:O     | 2.36                     | 0.74              |
| 12:L:30:ILE:O   | 12:L:56:LEU:HA   | 1.88                     | 0.74              |
| 1:A:344:ARG:C   | 2:B:1129:ARG:C   | 2.56                     | 0.73              |
| 2:B:1193:GLN:O  | 7:G:62:LEU:C     | 2.31                     | 0.73              |
| 2:B:411:PRO:O   | 2:B:414:ALA:HB3  | 1.88                     | 0.73              |
| 1:A:626:ASN:HA  | 1:A:1364:ASN:N   | 2.04                     | 0.73              |
| 2:B:1219:ASP:CB | 7:G:59:GLY:CA    | 2.66                     | 0.73              |
| 6:F:75:PRO:HA   | 7:G:26:LEU:N     | 2.03                     | 0.73              |
| 1:A:800:VAL:N   | 1:A:817:ALA:N    | 2.14                     | 0.73              |
| 1:A:504:LEU:O   | 1:A:1063:MET:CB  | 2.36                     | 0.73              |
| 1:A:1104:PRO:O  | 1:A:1105:SER:O   | 2.06                     | 0.73              |
| 2:B:1159:ARG:CA | 7:G:64:THR:CB    | 2.67                     | 0.73              |
| 1:A:491:VAL:C   | 2:B:1153:GLU:HA  | 2.14                     | 0.73              |
| 1:A:450:LEU:CA  | 1:A:843:LYS:H    | 2.01                     | 0.72              |
| 1:A:861:GLY:C   | 1:A:1420:ASP:CB  | 2.62                     | 0.72              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 8:H:36:CYS:HA   | 8:H:126:GLU:O    | 1.89                     | 0.72              |
| 2:B:642:ASP:O   | 2:B:644:GLU:N    | 2.22                     | 0.72              |
| 1:A:386:ASP:CB  | 6:F:104:ASN:CB   | 2.67                     | 0.72              |
| 4:D:130:LEU:O   | 4:D:132:GLN:N    | 2.22                     | 0.72              |
| 2:B:1148:LYS:N  | 2:B:1200:ALA:CB  | 2.52                     | 0.72              |
| 2:B:1224:PHE:CB | 5:E:175:LEU:HA   | 2.19                     | 0.72              |
| 1:A:862:ASN:CB  | 1:A:1420:ASP:CB  | 2.68                     | 0.72              |
| 2:B:1219:ASP:CA | 6:F:138:LEU:C    | 2.54                     | 0.72              |
| 3:C:263:THR:C   | 3:C:265:MET:H    | 1.97                     | 0.72              |
| 1:A:1427:ASN:N  | 2:B:1139:ILE:HA  | 1.64                     | 0.72              |
| 2:B:1149:GLU:CB | 2:B:1157:ALA:CA  | 2.68                     | 0.72              |
| 2:B:1219:ASP:CB | 7:G:59:GLY:N     | 2.52                     | 0.72              |
| 6:F:73:ALA:N    | 7:G:70:PHE:CB    | 2.52                     | 0.72              |
| 1:A:630:ILE:O   | 1:A:876:ALA:C    | 2.31                     | 0.72              |
| 1:A:69:THR:C    | 1:A:71:GLN:H     | 1.98                     | 0.71              |
| 1:A:608:ILE:CB  | 1:A:962:ARG:CB   | 2.67                     | 0.71              |
| 1:A:89:PRO:CA   | 4:D:16:LYS:CB    | 2.69                     | 0.71              |
| 2:B:1185:CYS:O  | 4:D:4:SER:N      | 2.23                     | 0.71              |
| 1:A:68:GLN:C    | 1:A:70:CYS:H     | 1.96                     | 0.71              |
| 2:B:1191:ILE:C  | 7:G:67:SER:CB    | 2.63                     | 0.71              |
| 1:A:1431:GLY:N  | 2:B:1147:LEU:N   | 2.34                     | 0.70              |
| 1:A:513:SER:HA  | 1:A:1067:LEU:CB  | 2.19                     | 0.70              |
| 1:A:862:ASN:O   | 1:A:1422:ARG:CB  | 2.38                     | 0.70              |
| 4:D:5:THR:O     | 4:D:6:SER:O      | 2.07                     | 0.70              |
| 4:D:176:GLU:C   | 4:D:178:ALA:H    | 1.98                     | 0.70              |
| 1:A:302:THR:HA  | 1:A:305:ASP:O    | 1.91                     | 0.70              |
| 1:A:509:LEU:CA  | 1:A:1062:GLU:HA  | 2.12                     | 0.70              |
| 1:A:846:GLU:CB  | 2:B:1140:ALA:HB2 | 2.16                     | 0.70              |
| 2:B:211:VAL:O   | 2:B:480:SER:HA   | 1.91                     | 0.70              |
| 2:B:708:GLU:O   | 2:B:710:LEU:N    | 2.25                     | 0.70              |
| 1:A:1445:ILE:N  | 2:B:1190:ASP:O   | 2.18                     | 0.70              |
| 1:A:1430:LEU:O  | 2:B:1147:LEU:N   | 2.23                     | 0.70              |
| 1:A:10:PRO:CB   | 7:G:15:PRO:N     | 2.55                     | 0.70              |
| 2:B:1194:ILE:O  | 7:G:64:THR:N     | 2.03                     | 0.70              |
| 1:A:9:ALA:HB3   | 7:G:65:ASP:CB    | 2.22                     | 0.69              |
| 1:A:766:GLY:O   | 1:A:817:ALA:O    | 2.10                     | 0.69              |
| 1:A:860:LEU:O   | 1:A:1419:ASP:O   | 2.10                     | 0.69              |
| 1:A:92:HIS:O    | 1:A:94:GLY:N     | 2.24                     | 0.69              |
| 2:B:1217:TYR:C  | 6:F:140:ASP:C    | 2.53                     | 0.69              |
| 1:A:766:GLY:N   | 1:A:820:GLY:H    | 1.89                     | 0.69              |
| 2:B:1099:VAL:O  | 2:B:1101:ASP:N   | 2.24                     | 0.69              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:B:1145:SER:C  | 2:B:1195:HIS:C   | 2.39                     | 0.69              |
| 8:H:4:THR:HA    | 8:H:60:ALA:CB    | 2.23                     | 0.69              |
| 1:A:800:VAL:H   | 1:A:817:ALA:N    | 1.89                     | 0.69              |
| 2:B:393:LYS:HA  | 9:I:90:GLN:O     | 1.76                     | 0.69              |
| 1:A:348:SER:CB  | 2:B:1154:ALA:O   | 2.39                     | 0.69              |
| 1:A:862:ASN:N   | 1:A:1420:ASP:CA  | 2.55                     | 0.69              |
| 1:A:635:ARG:O   | 1:A:1056:SER:CB  | 2.41                     | 0.69              |
| 2:B:1148:LYS:HA | 2:B:1200:ALA:H   | 1.57                     | 0.69              |
| 1:A:1430:LEU:C  | 2:B:1143:ALA:C   | 2.60                     | 0.69              |
| 2:B:847:ASP:C   | 2:B:849:GLY:H    | 1.99                     | 0.69              |
| 1:A:626:ASN:N   | 1:A:1362:TYR:O   | 2.26                     | 0.69              |
| 1:A:1430:LEU:O  | 2:B:1146:PHE:N   | 2.25                     | 0.69              |
| 2:B:1192:TYR:CB | 7:G:62:LEU:H     | 2.06                     | 0.69              |
| 1:A:1430:LEU:O  | 2:B:1145:SER:C   | 2.36                     | 0.68              |
| 1:A:514:PRO:CA  | 1:A:1367:HIS:HA  | 2.22                     | 0.68              |
| 1:A:19:PHE:O    | 1:A:1416:ALA:HA  | 1.93                     | 0.68              |
| 2:B:1145:SER:CA | 2:B:1195:HIS:C   | 2.66                     | 0.68              |
| 1:A:513:SER:O   | 1:A:1367:HIS:CA  | 2.41                     | 0.68              |
| 2:B:1145:SER:C  | 2:B:1195:HIS:O   | 2.28                     | 0.68              |
| 9:I:3:THR:O     | 9:I:42:LEU:C     | 2.37                     | 0.68              |
| 1:A:860:LEU:O   | 1:A:1440:ALA:HB2 | 1.93                     | 0.68              |
| 1:A:1448:GLU:HA | 7:G:32:GLU:N     | 2.07                     | 0.68              |
| 8:H:89:LEU:C    | 8:H:91:ASP:H     | 2.02                     | 0.68              |
| 1:A:451:HIS:N   | 1:A:843:LYS:N    | 2.41                     | 0.67              |
| 1:A:800:VAL:H   | 1:A:818:MET:N    | 1.92                     | 0.67              |
| 1:A:847:ASP:HA  | 2:B:1142:GLY:N   | 1.88                     | 0.67              |
| 2:B:1192:TYR:HA | 7:G:67:SER:CA    | 2.25                     | 0.67              |
| 2:B:1184:GLY:O  | 4:D:4:SER:CB     | 2.42                     | 0.67              |
| 1:A:1431:GLY:O  | 2:B:1146:PHE:CB  | 2.43                     | 0.67              |
| 1:A:233:TRP:O   | 4:D:13:ARG:O     | 1.93                     | 0.67              |
| 1:A:633:VAL:O   | 1:A:877:HIS:CB   | 2.43                     | 0.67              |
| 1:A:399:HIS:O   | 1:A:401:GLY:N    | 2.28                     | 0.66              |
| 1:A:778:GLY:C   | 2:B:402:GLY:H    | 2.03                     | 0.66              |
| 1:A:75:ASN:O    | 1:A:76:GLU:CB    | 2.43                     | 0.66              |
| 1:A:518:LYS:HA  | 1:A:1364:ASN:CB  | 2.25                     | 0.66              |
| 6:F:143:PHE:C   | 7:G:68:ALA:CB    | 2.68                     | 0.66              |
| 1:A:635:ARG:H   | 1:A:876:ALA:N    | 1.93                     | 0.66              |
| 1:A:862:ASN:H   | 1:A:1420:ASP:C   | 2.01                     | 0.66              |
| 6:F:135:ARG:CB  | 7:G:66:GLY:C     | 2.28                     | 0.66              |
| 2:B:1223:ASP:CB | 5:E:164:LEU:O    | 2.44                     | 0.66              |
| 1:A:69:THR:O    | 1:A:71:GLN:N     | 2.29                     | 0.66              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:1431:GLY:H   | 2:B:1147:LEU:CB | 2.08                     | 0.66              |
| 1:A:847:ASP:CA   | 2:B:1142:GLY:N  | 2.51                     | 0.65              |
| 6:F:73:ALA:HB3   | 7:G:11:ILE:CB   | 2.27                     | 0.65              |
| 1:A:1007:ILE:C   | 1:A:1009:ASN:H  | 2.02                     | 0.65              |
| 1:A:1391:ARG:O   | 1:A:1399:ARG:HA | 1.96                     | 0.65              |
| 5:E:176:PRO:O    | 5:E:212:ARG:HA  | 1.96                     | 0.65              |
| 4:D:176:GLU:O    | 4:D:178:ALA:N   | 2.26                     | 0.65              |
| 9:I:2:THR:O      | 9:I:3:THR:C     | 2.39                     | 0.65              |
| 2:B:1045:SER:O   | 2:B:1046:PRO:O  | 2.14                     | 0.65              |
| 6:F:135:ARG:CA   | 7:G:15:PRO:CB   | 2.75                     | 0.65              |
| 1:A:1424:VAL:O   | 2:B:1140:ALA:N  | 2.23                     | 0.65              |
| 4:D:156:ASP:C    | 4:D:158:GLU:H   | 2.03                     | 0.65              |
| 1:A:1065:GLY:CA  | 1:A:1435:PRO:C  | 2.70                     | 0.64              |
| 8:H:91:ASP:C     | 8:H:93:TYR:H    | 2.06                     | 0.64              |
| 1:A:626:ASN:N    | 1:A:1362:TYR:C  | 2.54                     | 0.64              |
| 1:A:1393:ASN:O   | 1:A:1397:LEU:N  | 2.21                     | 0.64              |
| 4:D:130:LEU:C    | 4:D:132:GLN:N   | 2.54                     | 0.64              |
| 2:B:357:GLN:O    | 2:B:366:GLN:HA  | 1.97                     | 0.64              |
| 1:A:346:ASP:O    | 2:B:1155:SER:O  | 2.16                     | 0.64              |
| 2:B:1195:HIS:N   | 7:G:63:PRO:CB   | 2.54                     | 0.64              |
| 2:B:642:ASP:HA   | 2:B:649:LYS:HA  | 1.77                     | 0.64              |
| 5:E:157:SER:C    | 5:E:159:ASP:H   | 2.03                     | 0.64              |
| 1:A:69:THR:C     | 1:A:71:GLN:N    | 2.55                     | 0.64              |
| 6:F:111:LEU:C    | 6:F:113:GLY:N   | 2.55                     | 0.64              |
| 10:J:23:ASN:C    | 10:J:25:LEU:H   | 2.05                     | 0.64              |
| 1:A:50:ILE:O     | 1:A:52:GLY:N    | 2.28                     | 0.64              |
| 1:A:340:LEU:O    | 2:B:1135:ARG:CB | 2.45                     | 0.64              |
| 1:A:1431:GLY:HA3 | 2:B:1146:PHE:CB | 2.28                     | 0.64              |
| 2:B:1099:VAL:C   | 2:B:1101:ASP:H  | 2.07                     | 0.64              |
| 3:C:168:ALA:O    | 3:C:170:TRP:N   | 2.30                     | 0.64              |
| 10:J:1:MET:H2    | 10:J:56:LEU:N   | 1.95                     | 0.64              |
| 1:A:384:ASN:O    | 1:A:385:ILE:C   | 2.41                     | 0.63              |
| 1:A:514:PRO:CA   | 1:A:1370:LEU:CB | 2.76                     | 0.63              |
| 1:A:766:GLY:O    | 1:A:817:ALA:CA  | 2.47                     | 0.63              |
| 6:F:77:ASP:H     | 7:G:23:LYS:CA   | 2.12                     | 0.63              |
| 1:A:235:ILE:O    | 4:D:15:LEU:C    | 2.26                     | 0.63              |
| 1:A:637:LYS:C    | 1:A:1055:ARG:O  | 2.41                     | 0.63              |
| 1:A:858:ASN:H    | 1:A:1422:ARG:CA | 2.05                     | 0.63              |
| 2:B:1184:GLY:O   | 4:D:4:SER:N     | 2.32                     | 0.63              |
| 1:A:4:GLN:O      | 1:A:5:GLN:O     | 2.17                     | 0.63              |
| 2:B:121:ASN:HA   | 2:B:207:GLY:CA  | 2.29                     | 0.63              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:C:99:LEU:HA   | 3:C:119:VAL:O    | 1.98                     | 0.63              |
| 1:A:227:VAL:O   | 4:D:10:THR:HA    | 1.96                     | 0.63              |
| 1:A:50:ILE:C    | 1:A:52:GLY:H     | 2.06                     | 0.62              |
| 1:A:383:TYR:O   | 6:F:105:ALA:HB2  | 1.98                     | 0.62              |
| 1:A:515:GLN:CB  | 1:A:1068:ALA:C   | 2.71                     | 0.62              |
| 4:D:191:ALA:O   | 4:D:193:THR:N    | 2.32                     | 0.62              |
| 1:A:135:PHE:C   | 1:A:137:ALA:H    | 2.06                     | 0.62              |
| 2:B:205:ILE:O   | 2:B:207:GLY:N    | 2.32                     | 0.62              |
| 2:B:1193:GLN:C  | 7:G:65:ASP:O     | 2.41                     | 0.62              |
| 3:C:31:ASN:O    | 3:C:32:SER:C     | 2.42                     | 0.62              |
| 2:B:121:ASN:HA  | 2:B:207:GLY:HA2  | 1.81                     | 0.62              |
| 2:B:1192:TYR:CA | 7:G:62:LEU:CB    | 2.77                     | 0.62              |
| 2:B:1222:ARG:CB | 5:E:171:LYS:H    | 1.27                     | 0.62              |
| 1:A:634:THR:C   | 1:A:877:HIS:N    | 2.58                     | 0.62              |
| 1:A:722:LEU:O   | 1:A:725:ALA:HB3  | 1.99                     | 0.62              |
| 6:F:142:SER:CB  | 7:G:70:PHE:HA    | 2.29                     | 0.62              |
| 1:A:289:ILE:C   | 1:A:291:GLU:H    | 2.07                     | 0.62              |
| 1:A:862:ASN:HA  | 1:A:1420:ASP:CB  | 2.27                     | 0.62              |
| 4:D:198:LEU:O   | 4:D:200:ASN:N    | 2.33                     | 0.62              |
| 1:A:10:PRO:N    | 7:G:67:SER:HA    | 2.13                     | 0.62              |
| 2:B:1159:ARG:C  | 7:G:64:THR:CB    | 2.73                     | 0.62              |
| 1:A:859:SER:N   | 1:A:1421:CYS:C   | 2.55                     | 0.61              |
| 1:A:1452:LYS:N  | 7:G:28:THR:CB    | 2.61                     | 0.61              |
| 2:B:745:PRO:C   | 2:B:747:MET:H    | 2.09                     | 0.61              |
| 1:A:518:LYS:CB  | 1:A:1363:VAL:C   | 2.73                     | 0.61              |
| 1:A:1393:ASN:CA | 1:A:1399:ARG:H   | 2.06                     | 0.61              |
| 1:A:453:MET:H   | 1:A:1066:VAL:CA  | 2.13                     | 0.61              |
| 1:A:1450:LEU:CB | 2:B:1189:ILE:CB  | 2.77                     | 0.61              |
| 1:A:384:ASN:O   | 1:A:386:ASP:N    | 2.34                     | 0.61              |
| 1:A:520:CYS:CB  | 1:A:1071:SER:H   | 2.11                     | 0.61              |
| 1:A:1431:GLY:C  | 2:B:1143:ALA:C   | 2.52                     | 0.61              |
| 2:B:745:PRO:O   | 2:B:747:MET:N    | 2.33                     | 0.61              |
| 3:C:39:ALA:CA   | 3:C:164:ALA:HB3  | 2.29                     | 0.61              |
| 2:B:1148:LYS:N  | 2:B:1200:ALA:HB3 | 2.02                     | 0.61              |
| 1:A:492:PRO:N   | 2:B:1153:GLU:HA  | 2.15                     | 0.61              |
| 1:A:774:ARG:O   | 1:A:775:ILE:C    | 2.43                     | 0.60              |
| 4:D:68:ARG:C    | 4:D:70:PHE:H     | 2.09                     | 0.60              |
| 6:F:143:PHE:CB  | 7:G:68:ALA:HB3   | 1.09                     | 0.60              |
| 12:L:36:SER:O   | 12:L:37:LYS:C    | 2.44                     | 0.60              |
| 6:F:143:PHE:CB  | 7:G:68:ALA:C     | 2.70                     | 0.60              |
| 6:F:73:ALA:HB2  | 7:G:11:ILE:O     | 2.01                     | 0.60              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1444:MET:CA | 2:B:1165:ILE:N   | 2.60                     | 0.60              |
| 2:B:1190:ASP:CB | 6:F:73:ALA:HB2   | 2.31                     | 0.60              |
| 3:C:208:GLU:O   | 3:C:210:GLU:N    | 2.34                     | 0.60              |
| 1:A:1431:GLY:N  | 2:B:1147:LEU:CA  | 2.64                     | 0.60              |
| 1:A:341:MET:O   | 2:B:1132:GLU:N   | 2.34                     | 0.60              |
| 1:A:520:CYS:HA  | 1:A:1071:SER:HA  | 1.84                     | 0.60              |
| 6:F:72:LYS:C    | 7:G:11:ILE:H     | 2.10                     | 0.60              |
| 1:A:237:THR:CB  | 4:D:16:LYS:HA    | 2.31                     | 0.60              |
| 2:B:1034:VAL:C  | 2:B:1036:ALA:H   | 2.10                     | 0.60              |
| 2:B:1148:LYS:CB | 2:B:1201:LYS:N   | 2.64                     | 0.59              |
| 1:A:862:ASN:CA  | 1:A:1422:ARG:CB  | 2.80                     | 0.59              |
| 1:A:1441:PHE:CB | 2:B:1217:TYR:C   | 2.75                     | 0.59              |
| 2:B:1180:PHE:O  | 2:B:1181:GLU:O   | 2.20                     | 0.59              |
| 3:C:254:LYS:O   | 3:C:256:ALA:N    | 2.35                     | 0.59              |
| 1:A:1017:LEU:CB | 5:E:205:SER:HA   | 2.33                     | 0.59              |
| 5:E:35:VAL:C    | 5:E:37:LEU:H     | 2.10                     | 0.59              |
| 6:F:77:ASP:C    | 6:F:79:ARG:H     | 2.10                     | 0.59              |
| 1:A:492:PRO:CA  | 2:B:1157:ALA:HB1 | 2.29                     | 0.59              |
| 8:H:83:GLN:C    | 8:H:85:GLY:H     | 2.08                     | 0.59              |
| 1:A:1313:LEU:O  | 1:A:1315:GLU:N   | 2.35                     | 0.59              |
| 6:F:72:LYS:N    | 7:G:69:GLU:HA    | 2.17                     | 0.59              |
| 2:B:446:LEU:O   | 2:B:447:ALA:HB3  | 2.02                     | 0.59              |
| 2:B:189:LEU:O   | 2:B:192:LEU:N    | 2.28                     | 0.59              |
| 2:B:265:SER:O   | 2:B:266:ALA:HB3  | 2.02                     | 0.59              |
| 1:A:71:GLN:C    | 1:A:73:GLY:H     | 2.09                     | 0.58              |
| 4:D:156:ASP:C   | 4:D:158:GLU:N    | 2.60                     | 0.58              |
| 1:A:262:LEU:O   | 1:A:264:PHE:N    | 2.37                     | 0.58              |
| 1:A:698:GLN:HA  | 9:I:97:MET:O     | 2.04                     | 0.58              |
| 4:D:191:ALA:C   | 4:D:193:THR:H    | 2.12                     | 0.58              |
| 2:B:1219:ASP:HA | 6:F:138:LEU:CA   | 2.33                     | 0.58              |
| 3:C:263:THR:C   | 3:C:265:MET:N    | 2.61                     | 0.58              |
| 2:B:640:VAL:O   | 2:B:641:GLU:C    | 2.46                     | 0.58              |
| 1:A:98:LYS:O    | 1:A:99:ILE:C     | 2.45                     | 0.58              |
| 1:A:262:LEU:C   | 1:A:264:PHE:H    | 2.11                     | 0.58              |
| 1:A:517:ASN:O   | 1:A:1365:TYR:C   | 2.45                     | 0.58              |
| 1:A:665:GLY:O   | 1:A:667:GLY:N    | 2.36                     | 0.58              |
| 6:F:142:SER:O   | 7:G:60:ARG:C     | 2.45                     | 0.58              |
| 1:A:801:GLU:HA  | 1:A:816:HIS:CB   | 2.33                     | 0.58              |
| 9:I:61:ASP:C    | 9:I:63:GLY:H     | 2.12                     | 0.58              |
| 1:A:35:ILE:HA   | 1:A:52:GLY:O     | 2.04                     | 0.58              |
| 1:A:311:GLN:O   | 1:A:312:PRO:C    | 2.47                     | 0.58              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:B:283:VAL:O   | 2:B:286:PHE:N   | 2.37                     | 0.58              |
| 5:E:90:VAL:HA   | 5:E:120:ALA:HB2 | 1.85                     | 0.58              |
| 1:A:848:ILE:O   | 1:A:1434:ALA:O  | 2.22                     | 0.57              |
| 1:A:513:SER:CA  | 1:A:1067:LEU:CB | 2.81                     | 0.57              |
| 1:A:800:VAL:N   | 1:A:818:MET:H   | 2.02                     | 0.57              |
| 9:I:14:LEU:HA   | 9:I:28:GLU:O    | 2.04                     | 0.57              |
| 1:A:61:ILE:O    | 1:A:63:ARG:N    | 2.38                     | 0.57              |
| 1:A:341:MET:C   | 2:B:1132:GLU:CA | 2.57                     | 0.57              |
| 1:A:635:ARG:H   | 1:A:875:ALA:C   | 2.11                     | 0.57              |
| 6:F:72:LYS:O    | 7:G:11:ILE:N    | 2.33                     | 0.57              |
| 6:F:135:ARG:HA  | 7:G:15:PRO:HA   | 1.86                     | 0.57              |
| 1:A:207:ILE:O   | 1:A:208:LEU:C   | 2.48                     | 0.57              |
| 2:B:224:GLN:O   | 2:B:238:ALA:HA  | 2.04                     | 0.57              |
| 2:B:1192:TYR:CB | 7:G:62:LEU:N    | 2.66                     | 0.57              |
| 1:A:15:LYS:N    | 1:A:1440:ALA:N  | 2.47                     | 0.57              |
| 1:A:77:CYS:O    | 1:A:78:PRO:C    | 2.40                     | 0.57              |
| 1:A:496:GLU:O   | 7:G:63:PRO:O    | 2.22                     | 0.57              |
| 1:A:848:ILE:O   | 1:A:1434:ALA:C  | 2.46                     | 0.57              |
| 2:B:957:ASN:O   | 2:B:959:ASP:N   | 2.37                     | 0.57              |
| 6:F:143:PHE:C   | 7:G:68:ALA:HB3  | 2.30                     | 0.57              |
| 1:A:1323:ASP:C  | 1:A:1325:THR:H  | 2.12                     | 0.57              |
| 2:B:1102:LYS:O  | 2:B:1103:ILE:C  | 2.47                     | 0.57              |
| 2:B:1192:TYR:CA | 7:G:67:SER:O    | 2.52                     | 0.57              |
| 1:A:545:GLN:O   | 1:A:546:VAL:C   | 2.46                     | 0.57              |
| 1:A:766:GLY:C   | 1:A:820:GLY:H   | 2.12                     | 0.57              |
| 1:A:799:PHE:C   | 1:A:815:PHE:C   | 2.63                     | 0.57              |
| 5:E:157:SER:C   | 5:E:159:ASP:N   | 2.60                     | 0.57              |
| 7:G:26:LEU:O    | 7:G:27:LYS:C    | 2.48                     | 0.57              |
| 1:A:14:VAL:CB   | 2:B:1144:ALA:CB | 2.83                     | 0.56              |
| 1:A:299:HIS:C   | 1:A:301:ALA:H   | 2.11                     | 0.56              |
| 1:A:1393:ASN:CA | 1:A:1399:ARG:N  | 2.65                     | 0.56              |
| 2:B:311:LEU:O   | 2:B:312:GLU:C   | 2.48                     | 0.56              |
| 3:C:76:ASP:O    | 3:C:77:ILE:C    | 2.48                     | 0.56              |
| 10:J:1:MET:N    | 10:J:56:LEU:N   | 2.53                     | 0.56              |
| 10:J:27:GLU:C   | 10:J:29:GLU:H   | 2.13                     | 0.56              |
| 1:A:386:ASP:CB  | 6:F:104:ASN:C   | 2.76                     | 0.56              |
| 1:A:598:LEU:O   | 1:A:599:SER:C   | 2.47                     | 0.56              |
| 1:A:840:ARG:O   | 1:A:841:LEU:C   | 2.47                     | 0.56              |
| 1:A:1007:ILE:C  | 1:A:1009:ASN:N  | 2.62                     | 0.56              |
| 1:A:1035:TYR:O  | 1:A:1037:LEU:N  | 2.37                     | 0.56              |
| 1:A:1396:ALA:O  | 1:A:1398:MET:N  | 2.38                     | 0.56              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:B:394:ASP:HA   | 9:I:92:ARG:C    | 2.30                     | 0.56              |
| 2:B:1146:PHE:O   | 2:B:1197:PRO:CB | 2.54                     | 0.56              |
| 1:A:513:SER:O    | 1:A:1367:HIS:HA | 2.04                     | 0.56              |
| 1:A:845:LEU:O    | 1:A:846:GLU:C   | 2.49                     | 0.56              |
| 1:A:1442:ASP:HA  | 2:B:1216:LEU:C  | 2.29                     | 0.56              |
| 1:A:1445:ILE:CB  | 2:B:1189:ILE:N  | 2.68                     | 0.56              |
| 3:C:27:LEU:O     | 3:C:28:ALA:C    | 2.47                     | 0.56              |
| 1:A:321:PRO:O    | 1:A:322:VAL:CB  | 2.53                     | 0.56              |
| 1:A:1393:ASN:O   | 1:A:1396:ALA:C  | 2.48                     | 0.56              |
| 1:A:64:ASN:O     | 1:A:65:LEU:C    | 2.48                     | 0.56              |
| 1:A:387:ARG:N    | 6:F:104:ASN:CA  | 2.66                     | 0.56              |
| 2:B:44:VAL:O     | 2:B:45:SER:C    | 2.49                     | 0.56              |
| 2:B:401:PHE:O    | 2:B:517:THR:N   | 2.34                     | 0.56              |
| 9:I:74:GLU:HA    | 9:I:80:SER:O    | 2.06                     | 0.56              |
| 1:A:482:PHE:C    | 1:A:484:GLY:H   | 2.13                     | 0.56              |
| 2:B:393:LYS:CA   | 9:I:90:GLN:O    | 2.40                     | 0.56              |
| 1:A:514:PRO:O    | 1:A:1370:LEU:CB | 2.53                     | 0.56              |
| 1:A:817:ALA:O    | 1:A:818:MET:C   | 2.48                     | 0.56              |
| 2:B:114:PRO:O    | 2:B:116:GLU:N   | 2.38                     | 0.56              |
| 2:B:1148:LYS:CA  | 2:B:1200:ALA:H  | 2.18                     | 0.56              |
| 2:B:1148:LYS:O   | 2:B:1200:ALA:N  | 2.39                     | 0.56              |
| 1:A:502:SER:O    | 6:F:88:TYR:CB   | 2.54                     | 0.55              |
| 2:B:1193:GLN:C   | 7:G:62:LEU:CB   | 2.80                     | 0.55              |
| 1:A:548:ASN:HA   | 11:K:60:ALA:HB1 | 1.89                     | 0.55              |
| 3:C:174:ALA:O    | 3:C:175:ALA:HB2 | 2.05                     | 0.55              |
| 1:A:630:ILE:O    | 1:A:876:ALA:O   | 2.24                     | 0.55              |
| 1:A:1157:ASP:C   | 1:A:1159:ARG:H  | 2.14                     | 0.55              |
| 2:B:773:MET:C    | 2:B:775:LYS:H   | 2.13                     | 0.55              |
| 1:A:829:VAL:C    | 1:A:831:THR:H   | 2.14                     | 0.55              |
| 1:A:847:ASP:CA   | 2:B:1142:GLY:H  | 2.18                     | 0.55              |
| 2:B:1148:LYS:CA  | 2:B:1200:ALA:CA | 2.69                     | 0.55              |
| 1:A:625:SER:CA   | 1:A:1362:TYR:O  | 2.50                     | 0.55              |
| 1:A:637:LYS:HA   | 1:A:1055:ARG:CB | 2.37                     | 0.55              |
| 1:A:730:GLY:O    | 1:A:732:LEU:N   | 2.40                     | 0.55              |
| 1:A:1431:GLY:HA3 | 2:B:1146:PHE:CA | 2.37                     | 0.55              |
| 3:C:215:GLU:O    | 3:C:216:GLY:C   | 2.50                     | 0.55              |
| 10:J:23:ASN:C    | 10:J:25:LEU:N   | 2.64                     | 0.55              |
| 1:A:520:CYS:CB   | 1:A:1071:SER:CA | 2.85                     | 0.55              |
| 2:B:552:MET:C    | 2:B:554:ILE:H   | 2.15                     | 0.55              |
| 5:E:128:PRO:HA   | 5:E:129:PRO:C   | 2.32                     | 0.55              |
| 2:B:129:PHE:HA   | 2:B:165:VAL:O   | 2.06                     | 0.55              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 4:D:51:ASN:O    | 4:D:52:LEU:O    | 2.25                     | 0.55              |
| 6:F:134:ILE:CA  | 7:G:15:PRO:CB   | 2.85                     | 0.55              |
| 1:A:16:GLU:N    | 6:F:139:PRO:O   | 2.40                     | 0.55              |
| 1:A:452:LYS:H   | 1:A:1066:VAL:HA | 1.71                     | 0.54              |
| 1:A:800:VAL:N   | 1:A:818:MET:N   | 2.55                     | 0.54              |
| 4:D:64:VAL:C    | 4:D:66:ARG:H    | 2.14                     | 0.54              |
| 8:H:84:ALA:C    | 8:H:86:ASP:H    | 2.15                     | 0.54              |
| 1:A:316:GLN:O   | 1:A:317:LYS:C   | 2.50                     | 0.54              |
| 1:A:1377:THR:O  | 1:A:1379:GLY:N  | 2.41                     | 0.54              |
| 2:B:1192:TYR:HA | 7:G:67:SER:O    | 2.06                     | 0.54              |
| 6:F:75:PRO:CA   | 7:G:26:LEU:CB   | 2.85                     | 0.54              |
| 1:A:12:ARG:C    | 7:G:61:ILE:O    | 2.50                     | 0.54              |
| 1:A:23:SER:O    | 1:A:24:PRO:C    | 2.48                     | 0.54              |
| 1:A:1393:ASN:CA | 1:A:1396:ALA:O  | 2.54                     | 0.54              |
| 2:B:125:SER:HA  | 2:B:171:PRO:HA  | 1.89                     | 0.54              |
| 3:C:168:ALA:C   | 3:C:170:TRP:H   | 2.16                     | 0.54              |
| 3:C:254:LYS:C   | 3:C:256:ALA:H   | 2.15                     | 0.54              |
| 1:A:861:GLY:C   | 1:A:1420:ASP:CA | 2.74                     | 0.54              |
| 1:A:50:ILE:C    | 1:A:52:GLY:N    | 2.64                     | 0.54              |
| 3:C:168:ALA:C   | 3:C:170:TRP:N   | 2.64                     | 0.54              |
| 7:G:117:GLN:C   | 7:G:119:LEU:H   | 2.15                     | 0.54              |
| 1:A:738:LYS:C   | 1:A:740:LEU:H   | 2.15                     | 0.54              |
| 6:F:73:ALA:CB   | 7:G:11:ILE:CB   | 2.86                     | 0.54              |
| 6:F:143:PHE:CB  | 7:G:68:ALA:HA   | 2.17                     | 0.54              |
| 1:A:1437:GLY:O  | 1:A:1439:GLY:N  | 2.23                     | 0.54              |
| 2:B:1040:ASN:O  | 2:B:1041:GLU:C  | 2.50                     | 0.54              |
| 10:J:44:TYR:HA  | 10:J:47:ARG:CB  | 2.37                     | 0.54              |
| 1:A:847:ASP:O   | 2:B:1142:GLY:N  | 2.41                     | 0.54              |
| 1:A:1428:VAL:CB | 2:B:1139:ILE:CB | 2.86                     | 0.54              |
| 2:B:1146:PHE:C  | 2:B:1196:ILE:C  | 2.75                     | 0.54              |
| 2:B:1146:PHE:CA | 2:B:1196:ILE:CA | 2.61                     | 0.54              |
| 2:B:1159:ARG:HA | 7:G:64:THR:CB   | 2.38                     | 0.54              |
| 1:A:92:HIS:O    | 1:A:95:PHE:N    | 2.34                     | 0.54              |
| 2:B:558:LEU:C   | 2:B:560:GLU:H   | 2.16                     | 0.54              |
| 2:B:1193:GLN:C  | 7:G:65:ASP:H    | 2.15                     | 0.54              |
| 1:A:1053:PHE:C  | 1:A:1055:ARG:H  | 2.15                     | 0.53              |
| 2:B:1068:GLY:O  | 2:B:1069:PHE:O  | 2.27                     | 0.53              |
| 4:D:24:ALA:HA   | 7:G:83:LYS:O    | 2.08                     | 0.53              |
| 12:L:34:CYS:O   | 12:L:35:SER:C   | 2.52                     | 0.53              |
| 1:A:9:ALA:O     | 7:G:66:GLY:N    | 2.39                     | 0.53              |
| 1:A:586:ILE:C   | 1:A:959:ASN:CB  | 2.80                     | 0.53              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:766:GLY:C   | 1:A:817:ALA:O    | 2.52                     | 0.53              |
| 1:A:809:THR:CA  | 2:B:729:ILE:CB   | 2.86                     | 0.53              |
| 2:B:1220:ARG:HA | 6:F:140:ASP:CB   | 2.37                     | 0.53              |
| 1:A:794:PRO:C   | 1:A:796:SER:H    | 2.15                     | 0.53              |
| 2:B:363:HIS:O   | 2:B:364:ILE:CB   | 2.56                     | 0.53              |
| 2:B:1096:ARG:O  | 2:B:1097:HIS:CB  | 2.56                     | 0.53              |
| 1:A:420:ARG:O   | 1:A:421:ALA:C    | 2.51                     | 0.53              |
| 1:A:453:MET:CB  | 1:A:1066:VAL:CB  | 2.86                     | 0.53              |
| 2:B:777:ALA:HA  | 2:B:1095:LEU:HA  | 1.90                     | 0.53              |
| 1:A:47:ARG:O    | 1:A:48:ALA:HB2   | 2.08                     | 0.53              |
| 2:B:312:GLU:H   | 9:I:46:HIS:CA    | 2.17                     | 0.53              |
| 2:B:1148:LYS:CA | 2:B:1200:ALA:HB2 | 1.96                     | 0.53              |
| 1:A:244:PRO:O   | 1:A:247:ARG:N    | 2.41                     | 0.53              |
| 1:A:1451:VAL:C  | 1:A:1453:TYR:H   | 2.16                     | 0.53              |
| 2:B:872:GLU:HA  | 2:B:915:THR:O    | 2.08                     | 0.53              |
| 1:A:262:LEU:C   | 1:A:264:PHE:N    | 2.66                     | 0.53              |
| 1:A:766:GLY:C   | 1:A:820:GLY:N    | 2.67                     | 0.53              |
| 5:E:161:LYS:C   | 5:E:163:GLU:H    | 2.17                     | 0.53              |
| 1:A:68:GLN:C    | 1:A:70:CYS:N     | 2.65                     | 0.53              |
| 1:A:299:HIS:C   | 1:A:301:ALA:N    | 2.67                     | 0.53              |
| 2:B:281:PRO:O   | 2:B:283:VAL:N    | 2.41                     | 0.53              |
| 2:B:847:ASP:C   | 2:B:849:GLY:N    | 2.61                     | 0.53              |
| 2:B:1194:ILE:O  | 7:G:64:THR:CB    | 2.57                     | 0.53              |
| 3:C:107:SER:C   | 3:C:109:SER:H    | 2.17                     | 0.53              |
| 6:F:141:GLY:C   | 7:G:69:GLU:O     | 2.51                     | 0.53              |
| 8:H:139:ASN:O   | 8:H:140:ALA:HB2  | 2.08                     | 0.53              |
| 1:A:516:SER:H   | 1:A:1367:HIS:C   | 2.14                     | 0.53              |
| 1:A:1007:ILE:O  | 1:A:1009:ASN:N   | 2.41                     | 0.53              |
| 2:B:205:ILE:O   | 2:B:206:ASN:C    | 2.52                     | 0.53              |
| 2:B:1184:GLY:C  | 4:D:4:SER:N      | 2.67                     | 0.53              |
| 12:L:52:GLY:O   | 12:L:53:HIS:C    | 2.52                     | 0.53              |
| 1:A:277:GLU:C   | 1:A:279:LEU:H    | 2.17                     | 0.53              |
| 2:B:1193:GLN:C  | 7:G:62:LEU:C     | 2.69                     | 0.53              |
| 1:A:438:ASP:O   | 1:A:439:ASN:CB   | 2.57                     | 0.52              |
| 1:A:618:GLU:O   | 1:A:620:LYS:N    | 2.42                     | 0.52              |
| 1:A:960:ILE:O   | 1:A:961:ARG:C    | 2.50                     | 0.52              |
| 8:H:113:ALA:HB1 | 8:H:125:LEU:O    | 2.09                     | 0.52              |
| 1:A:765:VAL:O   | 1:A:820:GLY:CA   | 2.57                     | 0.52              |
| 4:D:64:VAL:C    | 4:D:66:ARG:N     | 2.67                     | 0.52              |
| 8:H:59:ILE:O    | 8:H:60:ALA:HB3   | 2.10                     | 0.52              |
| 8:H:138:GLU:O   | 8:H:139:ASN:C    | 2.52                     | 0.52              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:817:ALA:O   | 1:A:819:GLY:N   | 2.41                     | 0.52              |
| 1:A:496:GLU:C   | 7:G:63:PRO:C    | 2.76                     | 0.52              |
| 2:B:1160:VAL:N  | 7:G:64:THR:CB   | 2.73                     | 0.52              |
| 5:E:55:ARG:C    | 5:E:57:MET:H    | 2.17                     | 0.52              |
| 6:F:135:ARG:CA  | 7:G:15:PRO:HA   | 2.39                     | 0.52              |
| 1:A:730:GLY:C   | 1:A:732:LEU:H   | 2.18                     | 0.52              |
| 2:B:1186:ASP:N  | 4:D:4:SER:N     | 2.54                     | 0.52              |
| 3:C:215:GLU:O   | 3:C:217:ASP:N   | 2.43                     | 0.52              |
| 3:C:242:GLN:C   | 3:C:244:VAL:H   | 2.18                     | 0.52              |
| 1:A:589:GLN:O   | 1:A:880:LYS:CB  | 2.58                     | 0.52              |
| 2:B:360:PHE:O   | 2:B:361:LEU:C   | 2.51                     | 0.52              |
| 2:B:383:ASN:O   | 2:B:384:ARG:C   | 2.53                     | 0.52              |
| 2:B:492:LEU:O   | 2:B:495:LEU:N   | 2.40                     | 0.52              |
| 1:A:356:ASP:O   | 1:A:358:ASN:N   | 2.42                     | 0.52              |
| 1:A:509:LEU:CB  | 1:A:1063:MET:H  | 2.23                     | 0.52              |
| 1:A:1164:PRO:O  | 1:A:1166:ASP:N  | 2.43                     | 0.52              |
| 1:A:1427:ASN:N  | 2:B:1139:ILE:CB | 2.72                     | 0.52              |
| 3:C:254:LYS:C   | 3:C:256:ALA:N   | 2.67                     | 0.52              |
| 1:A:921:GLY:O   | 1:A:922:ASP:C   | 2.53                     | 0.52              |
| 7:G:117:GLN:O   | 7:G:119:LEU:N   | 2.43                     | 0.52              |
| 2:B:1220:ARG:CA | 6:F:140:ASP:CB  | 2.87                     | 0.52              |
| 3:C:242:GLN:C   | 3:C:244:VAL:N   | 2.68                     | 0.52              |
| 1:A:452:LYS:HA  | 1:A:846:GLU:CB  | 2.40                     | 0.51              |
| 2:B:750:GLY:O   | 2:B:751:VAL:C   | 2.53                     | 0.51              |
| 1:A:367:PRO:HA  | 1:A:463:ILE:O   | 2.10                     | 0.51              |
| 1:A:514:PRO:O   | 1:A:1371:LEU:N  | 2.39                     | 0.51              |
| 1:A:648:ASN:O   | 1:A:649:ILE:C   | 2.53                     | 0.51              |
| 1:A:800:VAL:CA  | 1:A:814:PHE:O   | 1.68                     | 0.51              |
| 3:C:263:THR:O   | 3:C:265:MET:N   | 2.43                     | 0.51              |
| 1:A:730:GLY:C   | 1:A:732:LEU:N   | 2.67                     | 0.51              |
| 1:A:1377:THR:O  | 1:A:1378:GLN:C  | 2.54                     | 0.51              |
| 2:B:455:SER:O   | 2:B:456:GLY:C   | 2.52                     | 0.51              |
| 8:H:33:GLN:C    | 8:H:35:GLN:H    | 2.18                     | 0.51              |
| 3:C:39:ALA:HA   | 3:C:164:ALA:CB  | 2.31                     | 0.51              |
| 8:H:84:ALA:C    | 8:H:86:ASP:N    | 2.67                     | 0.51              |
| 1:A:63:ARG:CA   | 1:A:411:ASP:CA  | 2.76                     | 0.51              |
| 1:A:129:LYS:CB  | 5:E:192:ARG:C   | 2.74                     | 0.51              |
| 2:B:765:PRO:O   | 2:B:768:THR:N   | 2.44                     | 0.51              |
| 2:B:1147:LEU:N  | 2:B:1197:PRO:N  | 2.56                     | 0.51              |
| 3:C:239:PRO:O   | 3:C:241:ASP:N   | 2.43                     | 0.51              |
| 6:F:72:LYS:C    | 7:G:70:PHE:CB   | 2.82                     | 0.51              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 6:F:77:ASP:C    | 6:F:79:ARG:N     | 2.67                     | 0.51              |
| 8:H:82:PRO:C    | 8:H:84:ALA:H     | 2.17                     | 0.51              |
| 1:A:418:SER:O   | 1:A:420:ARG:N    | 2.43                     | 0.51              |
| 1:A:516:SER:H   | 1:A:1367:HIS:CA  | 2.24                     | 0.51              |
| 2:B:745:PRO:C   | 2:B:747:MET:N    | 2.68                     | 0.51              |
| 1:A:335:ARG:O   | 1:A:336:ILE:C    | 2.52                     | 0.51              |
| 5:E:161:LYS:C   | 5:E:163:GLU:N    | 2.68                     | 0.51              |
| 8:H:27:GLU:HA   | 8:H:38:LEU:O     | 2.11                     | 0.51              |
| 1:A:95:PHE:O    | 1:A:96:ILE:C     | 2.53                     | 0.51              |
| 2:B:773:MET:C   | 2:B:775:LYS:N    | 2.65                     | 0.51              |
| 2:B:1174:LYS:O  | 2:B:1175:LEU:C   | 2.53                     | 0.51              |
| 1:A:82:GLY:O    | 1:A:241:VAL:N    | 2.42                     | 0.51              |
| 1:A:577:ILE:C   | 1:A:579:SER:N    | 2.65                     | 0.51              |
| 2:B:1107:ALA:O  | 2:B:1108:ARG:O   | 2.28                     | 0.51              |
| 2:B:1149:GLU:CB | 2:B:1157:ALA:HA  | 2.40                     | 0.51              |
| 2:B:1222:ARG:CB | 5:E:171:LYS:N    | 0.66                     | 0.51              |
| 1:A:450:LEU:HA  | 1:A:843:LYS:H    | 1.75                     | 0.50              |
| 1:A:984:LYS:O   | 1:A:985:ASP:C    | 2.54                     | 0.50              |
| 1:A:1017:LEU:CB | 5:E:206:GLY:H    | 2.23                     | 0.50              |
| 1:A:1334:ASP:O  | 1:A:1336:MET:N   | 2.43                     | 0.50              |
| 1:A:1369:ALA:O  | 1:A:1370:LEU:C   | 2.52                     | 0.50              |
| 2:B:642:ASP:CB  | 2:B:649:LYS:HA   | 2.41                     | 0.50              |
| 2:B:843:GLN:O   | 2:B:844:SER:C    | 2.54                     | 0.50              |
| 10:J:32:GLU:O   | 10:J:34:THR:N    | 2.45                     | 0.50              |
| 1:A:600:PRO:C   | 1:A:602:ASP:H    | 2.19                     | 0.50              |
| 8:H:62:SER:O    | 8:H:63:LEU:C     | 2.54                     | 0.50              |
| 1:A:71:GLN:C    | 1:A:73:GLY:N     | 2.69                     | 0.50              |
| 1:A:365:GLY:O   | 1:A:468:PHE:HA   | 2.10                     | 0.50              |
| 4:D:206:GLU:C   | 4:D:208:GLU:N    | 2.68                     | 0.50              |
| 1:A:26:GLU:O    | 1:A:27:VAL:C     | 2.54                     | 0.50              |
| 1:A:58:LEU:O    | 1:A:59:GLY:O     | 2.30                     | 0.50              |
| 1:A:317:LYS:O   | 1:A:318:SER:CB   | 2.60                     | 0.50              |
| 1:A:845:LEU:O   | 2:B:1140:ALA:HB1 | 2.08                     | 0.50              |
| 1:A:823:GLY:O   | 1:A:825:ILE:N    | 2.44                     | 0.50              |
| 2:B:1221:SER:O  | 5:E:165:LEU:O    | 2.30                     | 0.50              |
| 3:C:140:ASN:O   | 3:C:141:GLY:O    | 2.30                     | 0.50              |
| 1:A:496:GLU:O   | 2:B:1195:HIS:CB  | 2.52                     | 0.50              |
| 1:A:626:ASN:O   | 1:A:628:GLY:N    | 2.44                     | 0.50              |
| 1:A:802:ASN:H   | 1:A:813:PHE:CB   | 2.24                     | 0.50              |
| 3:C:213:PRO:O   | 3:C:214:ASN:CB   | 2.60                     | 0.50              |
| 1:A:28:ARG:O    | 1:A:29:ALA:C     | 2.55                     | 0.50              |

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| Atom-1         | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 1:A:755:PHE:O  | 1:A:756:ILE:C    | 2.55                     | 0.50              |
| 1:A:1280:GLU:O | 1:A:1281:ARG:C   | 2.55                     | 0.50              |
| 1:A:1445:ILE:N | 7:G:10:ASN:O     | 2.44                     | 0.50              |
| 3:C:33:LEU:O   | 3:C:34:ARG:C     | 2.54                     | 0.50              |
| 3:C:163:ILE:O  | 3:C:165:LYS:N    | 2.45                     | 0.50              |
| 1:A:450:LEU:O  | 1:A:843:LYS:N    | 2.40                     | 0.50              |
| 1:A:802:ASN:N  | 1:A:813:PHE:CB   | 2.70                     | 0.50              |
| 2:B:642:ASP:CA | 2:B:649:LYS:HA   | 2.42                     | 0.50              |
| 2:B:785:TYR:C  | 2:B:787:VAL:H    | 2.19                     | 0.50              |
| 10:J:27:GLU:O  | 10:J:29:GLU:N    | 2.45                     | 0.50              |
| 1:A:442:VAL:O  | 1:A:457:ALA:HA   | 2.12                     | 0.50              |
| 2:B:377:PHE:C  | 2:B:379:GLY:N    | 2.62                     | 0.50              |
| 2:B:1182:CYS:O | 2:B:1183:LYS:C   | 2.54                     | 0.50              |
| 2:B:1174:LYS:O | 2:B:1176:ASN:N   | 2.44                     | 0.49              |
| 1:A:68:GLN:O   | 1:A:70:CYS:N     | 2.43                     | 0.49              |
| 1:A:512:VAL:HA | 1:A:519:PRO:HA   | 1.93                     | 0.49              |
| 1:A:909:ASP:O  | 1:A:911:SER:N    | 2.45                     | 0.49              |
| 2:B:890:TYR:O  | 2:B:892:LYS:N    | 2.45                     | 0.49              |
| 1:A:116:ASP:O  | 1:A:118:HIS:N    | 2.45                     | 0.49              |
| 1:A:341:MET:O  | 2:B:1135:ARG:CB  | 2.60                     | 0.49              |
| 1:A:635:ARG:N  | 1:A:876:ALA:N    | 2.59                     | 0.49              |
| 1:A:1451:VAL:C | 1:A:1453:TYR:N   | 2.70                     | 0.49              |
| 3:C:142:VAL:H  | 10:J:16:ASP:CB   | 2.24                     | 0.49              |
| 7:G:117:GLN:C  | 7:G:119:LEU:N    | 2.69                     | 0.49              |
| 2:B:1148:LYS:N | 2:B:1200:ALA:HB2 | 2.24                     | 0.49              |
| 3:C:90:ASP:O   | 3:C:91:HIS:CB    | 2.60                     | 0.49              |
| 1:A:402:ALA:CB | 1:A:434:ARG:HA   | 2.43                     | 0.49              |
| 1:A:509:LEU:CB | 1:A:1063:MET:N   | 2.75                     | 0.49              |
| 3:C:256:ALA:C  | 3:C:258:ILE:H    | 2.19                     | 0.49              |
| 5:E:18:THR:O   | 5:E:19:VAL:C     | 2.55                     | 0.49              |
| 1:A:244:PRO:O  | 1:A:246:VAL:N    | 2.46                     | 0.49              |
| 1:A:1280:GLU:O | 1:A:1281:ARG:O   | 2.30                     | 0.49              |
| 1:A:1430:LEU:C | 2:B:1147:LEU:CA  | 2.85                     | 0.49              |
| 3:C:63:ILE:O   | 3:C:64:ALA:C     | 2.55                     | 0.49              |
| 9:I:2:THR:O    | 9:I:44:TYR:N     | 2.44                     | 0.49              |
| 3:C:77:ILE:O   | 3:C:79:GLN:N     | 2.46                     | 0.49              |
| 1:A:17:VAL:CA  | 1:A:1439:GLY:O   | 2.56                     | 0.49              |
| 1:A:332:LYS:O  | 1:A:334:GLY:N    | 2.46                     | 0.49              |
| 1:A:1388:GLY:O | 1:A:1390:ASN:N   | 2.46                     | 0.49              |
| 2:B:734:HIS:O  | 2:B:735:ALA:HB2  | 2.12                     | 0.49              |
| 1:A:452:LYS:CB | 1:A:1066:VAL:HA  | 2.34                     | 0.49              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:545:GLN:O   | 1:A:548:ASN:N   | 2.45                     | 0.49              |
| 1:A:809:THR:HA  | 2:B:729:ILE:CB  | 2.43                     | 0.49              |
| 2:B:511:PRO:O   | 2:B:512:ARG:C   | 2.54                     | 0.49              |
| 2:B:661:LEU:C   | 2:B:663:ALA:H   | 2.19                     | 0.49              |
| 2:B:1081:LEU:O  | 2:B:1082:MET:C  | 2.55                     | 0.49              |
| 4:D:135:GLY:C   | 4:D:137:ASN:H   | 2.21                     | 0.49              |
| 1:A:218:ASP:O   | 1:A:219:PHE:C   | 2.56                     | 0.49              |
| 1:A:1442:ASP:C  | 6:F:141:GLY:HA3 | 2.38                     | 0.49              |
| 6:F:77:ASP:HA   | 7:G:21:ARG:HA   | 1.95                     | 0.49              |
| 12:L:49:LYS:O   | 12:L:50:ASP:CB  | 2.60                     | 0.49              |
| 1:A:966:ASN:O   | 1:A:967:ALA:C   | 2.56                     | 0.48              |
| 1:A:1001:ARG:O  | 1:A:1002:GLY:O  | 2.31                     | 0.48              |
| 1:A:1424:VAL:HA | 2:B:1140:ALA:HA | 1.94                     | 0.48              |
| 2:B:954:VAL:O   | 12:L:55:ILE:O   | 2.31                     | 0.48              |
| 6:F:72:LYS:O    | 7:G:11:ILE:CB   | 2.61                     | 0.48              |
| 1:A:120:GLU:C   | 1:A:122:MET:N   | 2.70                     | 0.48              |
| 1:A:232:GLU:O   | 4:D:14:ARG:N    | 2.44                     | 0.48              |
| 1:A:243:PRO:O   | 1:A:244:PRO:C   | 2.55                     | 0.48              |
| 1:A:845:LEU:O   | 1:A:1434:ALA:C  | 2.56                     | 0.48              |
| 3:C:77:ILE:C    | 3:C:79:GLN:H    | 2.20                     | 0.48              |
| 3:C:105:GLY:O   | 3:C:149:LYS:O   | 2.32                     | 0.48              |
| 7:G:15:PRO:O    | 7:G:16:SER:C    | 2.55                     | 0.48              |
| 1:A:135:PHE:C   | 1:A:137:ALA:N   | 2.70                     | 0.48              |
| 1:A:626:ASN:C   | 1:A:628:GLY:H   | 2.21                     | 0.48              |
| 1:A:1444:MET:CA | 7:G:10:ASN:C    | 2.82                     | 0.48              |
| 2:B:125:SER:HA  | 2:B:172:ILE:H   | 1.78                     | 0.48              |
| 2:B:661:LEU:C   | 2:B:663:ALA:N   | 2.71                     | 0.48              |
| 9:I:3:THR:HA    | 9:I:45:ARG:N    | 2.21                     | 0.48              |
| 1:A:299:HIS:O   | 1:A:301:ALA:N   | 2.46                     | 0.48              |
| 1:A:766:GLY:C   | 1:A:817:ALA:C   | 2.73                     | 0.48              |
| 2:B:1193:GLN:CA | 7:G:62:LEU:CB   | 2.90                     | 0.48              |
| 8:H:82:PRO:O    | 8:H:84:ALA:N    | 2.35                     | 0.48              |
| 1:A:309:ALA:C   | 1:A:311:GLN:H   | 2.21                     | 0.48              |
| 1:A:514:PRO:C   | 1:A:1370:LEU:CB | 2.87                     | 0.48              |
| 2:B:563:MET:HA  | 2:B:589:VAL:O   | 2.13                     | 0.48              |
| 1:A:1431:GLY:CA | 2:B:1147:LEU:CA | 2.91                     | 0.48              |
| 2:B:1034:VAL:O  | 2:B:1036:ALA:N  | 2.46                     | 0.48              |
| 2:B:1177:HIS:C  | 2:B:1179:GLN:H  | 2.21                     | 0.48              |
| 7:G:66:GLY:O    | 7:G:67:SER:C    | 2.56                     | 0.48              |
| 8:H:91:ASP:C    | 8:H:93:TYR:N    | 2.72                     | 0.48              |
| 1:A:254:GLU:O   | 1:A:256:GLN:N   | 2.47                     | 0.48              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:325:ILE:O   | 1:A:326:ARG:C    | 2.55                     | 0.48              |
| 1:A:1073:GLY:O  | 1:A:1076:ALA:HB3 | 2.13                     | 0.48              |
| 2:B:98:THR:O    | 2:B:126:SER:CB   | 2.62                     | 0.48              |
| 2:B:552:MET:C   | 2:B:554:ILE:N    | 2.72                     | 0.48              |
| 2:B:847:ASP:O   | 2:B:849:GLY:N    | 2.47                     | 0.48              |
| 1:A:41:MET:O    | 1:A:42:ASP:C     | 2.56                     | 0.48              |
| 4:D:20:GLU:O    | 4:D:21:GLU:O     | 2.32                     | 0.48              |
| 4:D:146:GLN:O   | 4:D:147:TYR:C    | 2.57                     | 0.48              |
| 5:E:35:VAL:C    | 5:E:37:LEU:N     | 2.72                     | 0.48              |
| 1:A:10:PRO:O    | 7:G:65:ASP:C     | 2.55                     | 0.48              |
| 2:B:391:ASP:CB  | 9:I:94:ASP:CB    | 2.91                     | 0.48              |
| 3:C:82:TYR:O    | 3:C:83:SER:C     | 2.54                     | 0.48              |
| 10:J:32:GLU:O   | 10:J:35:ALA:N    | 2.46                     | 0.48              |
| 1:A:166:GLY:O   | 1:A:167:CYS:CB   | 2.62                     | 0.48              |
| 1:A:237:THR:CB  | 4:D:16:LYS:CA    | 2.92                     | 0.48              |
| 2:B:27:ALA:O    | 2:B:29:ASP:N     | 2.47                     | 0.48              |
| 6:F:145:ASP:CB  | 7:G:14:HIS:O     | 2.62                     | 0.48              |
| 6:F:73:ALA:CB   | 7:G:11:ILE:O     | 2.62                     | 0.47              |
| 1:A:800:VAL:CA  | 1:A:814:PHE:CA   | 2.71                     | 0.47              |
| 1:A:1015:VAL:O  | 1:A:1016:THR:C   | 2.57                     | 0.47              |
| 1:A:1445:ILE:CB | 2:B:1189:ILE:H   | 2.26                     | 0.47              |
| 2:B:1148:LYS:CB | 2:B:1201:LYS:H   | 2.27                     | 0.47              |
| 1:A:652:VAL:O   | 1:A:653:VAL:C    | 2.56                     | 0.47              |
| 1:A:1053:PHE:C  | 1:A:1055:ARG:N   | 2.70                     | 0.47              |
| 2:B:1148:LYS:CB | 2:B:1200:ALA:CA  | 2.86                     | 0.47              |
| 1:A:636:GLU:CB  | 1:A:877:HIS:C    | 2.83                     | 0.47              |
| 1:A:823:GLY:C   | 1:A:825:ILE:N    | 2.72                     | 0.47              |
| 2:B:394:ASP:N   | 9:I:92:ARG:C     | 2.73                     | 0.47              |
| 3:C:183:TRP:O   | 3:C:185:LYS:N    | 2.48                     | 0.47              |
| 7:G:44:TYR:O    | 7:G:78:VAL:HA    | 2.14                     | 0.47              |
| 8:H:4:THR:CA    | 8:H:60:ALA:HB2   | 2.34                     | 0.47              |
| 3:C:170:TRP:O   | 3:C:171:GLY:C    | 2.57                     | 0.47              |
| 4:D:191:ALA:C   | 4:D:193:THR:N    | 2.73                     | 0.47              |
| 10:J:16:ASP:O   | 10:J:18:TRP:N    | 2.47                     | 0.47              |
| 1:A:1265:ASN:C  | 1:A:1267:MET:N   | 2.67                     | 0.47              |
| 4:D:206:GLU:C   | 4:D:208:GLU:H    | 2.23                     | 0.47              |
| 6:F:135:ARG:CA  | 7:G:15:PRO:CA    | 2.92                     | 0.47              |
| 8:H:91:ASP:O    | 8:H:93:TYR:N     | 2.46                     | 0.47              |
| 8:H:99:GLY:HA3  | 8:H:118:PHE:HA   | 1.95                     | 0.47              |
| 9:I:61:ASP:O    | 9:I:63:GLY:N     | 2.48                     | 0.47              |
| 1:A:42:ASP:O    | 1:A:44:THR:N     | 2.45                     | 0.47              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:116:ASP:O   | 1:A:117:GLU:C   | 2.57                     | 0.47              |
| 1:A:289:ILE:C   | 1:A:291:GLU:N   | 2.73                     | 0.47              |
| 1:A:324:SER:O   | 1:A:325:ILE:C   | 2.56                     | 0.47              |
| 1:A:387:ARG:CA  | 6:F:104:ASN:CB  | 2.88                     | 0.47              |
| 1:A:496:GLU:O   | 1:A:499:ALA:HB3 | 2.15                     | 0.47              |
| 1:A:847:ASP:HA  | 2:B:1142:GLY:H  | 1.58                     | 0.47              |
| 1:A:1340:GLY:O  | 1:A:1343:ALA:N  | 2.43                     | 0.47              |
| 1:A:1344:GLY:O  | 1:A:1345:ARG:C  | 2.56                     | 0.47              |
| 2:B:192:LEU:O   | 2:B:193:LYS:CB  | 2.62                     | 0.47              |
| 2:B:558:LEU:O   | 2:B:560:GLU:N   | 2.47                     | 0.47              |
| 2:B:1208:MET:O  | 2:B:1211:ASN:N  | 2.40                     | 0.47              |
| 5:E:205:SER:O   | 5:E:206:GLY:C   | 2.58                     | 0.47              |
| 6:F:74:ILE:C    | 7:G:26:LEU:CB   | 2.87                     | 0.47              |
| 10:J:56:LEU:O   | 10:J:59:LYS:N   | 2.45                     | 0.47              |
| 11:K:52:ASN:O   | 11:K:54:ARG:N   | 2.48                     | 0.47              |
| 1:A:636:GLU:CB  | 1:A:877:HIS:O   | 2.62                     | 0.47              |
| 2:B:654:ARG:C   | 2:B:656:GLY:H   | 2.23                     | 0.47              |
| 2:B:1192:TYR:CB | 7:G:62:LEU:CA   | 2.90                     | 0.47              |
| 4:D:138:ASN:C   | 4:D:140:ASP:N   | 2.70                     | 0.47              |
| 5:E:129:PRO:O   | 5:E:130:ALA:C   | 2.57                     | 0.47              |
| 1:A:65:LEU:O    | 1:A:66:LYS:C    | 2.57                     | 0.47              |
| 2:B:20:ASP:O    | 2:B:22:SER:N    | 2.45                     | 0.47              |
| 2:B:225:VAL:HA  | 2:B:237:VAL:O   | 2.14                     | 0.47              |
| 4:D:176:GLU:C   | 4:D:178:ALA:N   | 2.63                     | 0.47              |
| 5:E:35:VAL:O    | 5:E:37:LEU:N    | 2.48                     | 0.47              |
| 5:E:55:ARG:C    | 5:E:57:MET:N    | 2.69                     | 0.47              |
| 1:A:279:LEU:O   | 1:A:284:ALA:HB2 | 2.15                     | 0.47              |
| 1:A:1334:ASP:C  | 1:A:1336:MET:H  | 2.23                     | 0.47              |
| 1:A:1449:SER:N  | 7:G:27:LYS:C    | 2.73                     | 0.47              |
| 3:C:253:LYS:O   | 3:C:256:ALA:HB3 | 2.15                     | 0.47              |
| 8:H:83:GLN:C    | 8:H:85:GLY:N    | 2.73                     | 0.47              |
| 2:B:591:ARG:O   | 2:B:592:ASN:C   | 2.57                     | 0.46              |
| 2:B:1146:PHE:O  | 2:B:1197:PRO:HA | 2.12                     | 0.46              |
| 4:D:68:ARG:C    | 4:D:70:PHE:N    | 2.70                     | 0.46              |
| 6:F:135:ARG:N   | 7:G:15:PRO:CA   | 2.74                     | 0.46              |
| 1:A:237:THR:CA  | 4:D:16:LYS:HA   | 2.45                     | 0.46              |
| 2:B:834:ASN:HA  | 2:B:838:SER:O   | 2.15                     | 0.46              |
| 3:C:208:GLU:C   | 3:C:210:GLU:H   | 2.22                     | 0.46              |
| 4:D:51:ASN:O    | 4:D:52:LEU:C    | 2.57                     | 0.46              |
| 10:J:23:ASN:O   | 10:J:25:LEU:N   | 2.49                     | 0.46              |
| 1:A:8:SER:O     | 7:G:14:HIS:CB   | 2.63                     | 0.46              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:298:PHE:O   | 1:A:301:ALA:HB3 | 2.15                     | 0.46              |
| 1:A:402:ALA:HB1 | 1:A:433:GLU:O   | 2.15                     | 0.46              |
| 1:A:1122:LYS:O  | 1:A:1124:ILE:N  | 2.49                     | 0.46              |
| 2:B:1152:MET:O  | 2:B:1154:ALA:N  | 2.49                     | 0.46              |
| 10:J:31:ASP:O   | 10:J:32:GLU:C   | 2.58                     | 0.46              |
| 1:A:277:GLU:C   | 1:A:279:LEU:N   | 2.74                     | 0.46              |
| 2:B:414:ALA:O   | 2:B:415:GLN:C   | 2.57                     | 0.46              |
| 1:A:509:LEU:CB  | 1:A:1062:GLU:C  | 2.82                     | 0.46              |
| 1:A:829:VAL:C   | 1:A:831:THR:N   | 2.74                     | 0.46              |
| 1:A:1410:PHE:C  | 1:A:1412:ALA:H  | 2.23                     | 0.46              |
| 2:B:1131:GLY:O  | 2:B:1132:GLU:C  | 2.58                     | 0.46              |
| 1:A:7:SER:C     | 1:A:9:ALA:H     | 2.23                     | 0.46              |
| 1:A:452:LYS:CA  | 1:A:1066:VAL:CB | 2.92                     | 0.46              |
| 1:A:452:LYS:N   | 1:A:1066:VAL:HA | 2.30                     | 0.46              |
| 1:A:859:SER:CB  | 2:B:1139:ILE:O  | 2.62                     | 0.46              |
| 1:A:935:GLN:C   | 1:A:937:VAL:N   | 2.72                     | 0.46              |
| 1:A:1027:ALA:O  | 1:A:1028:THR:C  | 2.59                     | 0.46              |
| 1:A:1334:ASP:C  | 1:A:1336:MET:N  | 2.74                     | 0.46              |
| 2:B:1178:ASN:O  | 2:B:1179:GLN:C  | 2.56                     | 0.46              |
| 3:C:47:ASP:CA   | 12:L:69:ALA:CB  | 2.87                     | 0.46              |
| 9:I:56:ALA:O    | 9:I:57:GLY:O    | 2.34                     | 0.46              |
| 11:K:59:ALA:HA  | 11:K:74:ARG:O   | 2.15                     | 0.46              |
| 2:B:681:TRP:O   | 2:B:683:SER:N   | 2.49                     | 0.46              |
| 4:D:51:ASN:C    | 4:D:52:LEU:O    | 2.59                     | 0.46              |
| 6:F:123:LYS:O   | 6:F:124:GLU:C   | 2.58                     | 0.46              |
| 11:K:113:THR:O  | 11:K:114:LEU:CB | 2.62                     | 0.46              |
| 1:A:43:GLU:O    | 1:A:44:THR:CB   | 2.64                     | 0.46              |
| 1:A:70:CYS:O    | 1:A:71:GLN:C    | 2.59                     | 0.46              |
| 1:A:935:GLN:O   | 1:A:936:LEU:C   | 2.59                     | 0.46              |
| 1:A:1428:VAL:O  | 2:B:1147:LEU:CB | 2.64                     | 0.46              |
| 2:B:558:LEU:C   | 2:B:560:GLU:N   | 2.74                     | 0.46              |
| 2:B:708:GLU:O   | 2:B:709:ASP:C   | 2.58                     | 0.46              |
| 2:B:1002:THR:O  | 2:B:1003:ALA:C  | 2.59                     | 0.46              |
| 2:B:1099:VAL:C  | 2:B:1101:ASP:N  | 2.70                     | 0.46              |
| 4:D:19:GLU:O    | 4:D:21:GLU:N    | 2.49                     | 0.46              |
| 6:F:77:ASP:H    | 7:G:23:LYS:C    | 2.23                     | 0.46              |
| 1:A:231:PRO:C   | 1:A:233:TRP:N   | 2.73                     | 0.46              |
| 1:A:427:GLN:O   | 1:A:428:TYR:C   | 2.56                     | 0.46              |
| 1:A:1019:CYS:O  | 1:A:1022:LEU:N  | 2.48                     | 0.46              |
| 2:B:785:TYR:C   | 2:B:787:VAL:N   | 2.71                     | 0.46              |
| 2:B:873:THR:O   | 2:B:914:LYS:HA  | 2.16                     | 0.46              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:B:1068:GLY:O  | 2:B:1069:PHE:C   | 2.59                     | 0.46              |
| 3:C:38:ILE:HA   | 3:C:173:ALA:HB2  | 1.98                     | 0.46              |
| 5:E:129:PRO:O   | 5:E:130:ALA:O    | 2.34                     | 0.46              |
| 1:A:341:MET:O   | 2:B:1131:GLY:C   | 2.59                     | 0.46              |
| 1:A:347:PHE:H   | 2:B:1107:ALA:HA  | 1.80                     | 0.46              |
| 1:A:356:ASP:C   | 1:A:358:ASN:H    | 2.24                     | 0.46              |
| 1:A:964:ILE:O   | 1:A:965:GLN:C    | 2.59                     | 0.46              |
| 2:B:48:LEU:O    | 2:B:49:ASP:C     | 2.59                     | 0.46              |
| 2:B:390:LEU:O   | 2:B:391:ASP:C    | 2.58                     | 0.46              |
| 3:C:236:GLY:C   | 3:C:238:ILE:N    | 2.73                     | 0.46              |
| 5:E:157:SER:O   | 5:E:159:ASP:N    | 2.48                     | 0.46              |
| 6:F:138:LEU:N   | 7:G:59:GLY:O     | 2.49                     | 0.46              |
| 7:G:13:LEU:O    | 7:G:67:SER:HA    | 2.15                     | 0.46              |
| 1:A:577:ILE:O   | 1:A:578:LEU:C    | 2.56                     | 0.45              |
| 1:A:1156:PRO:HA | 1:A:1190:PRO:CB  | 2.46                     | 0.45              |
| 1:A:1446:ASP:CB | 7:G:11:ILE:CB    | 2.64                     | 0.45              |
| 2:B:1148:LYS:CB | 2:B:1200:ALA:HB1 | 2.29                     | 0.45              |
| 4:D:196:PRO:C   | 4:D:198:LEU:H    | 2.23                     | 0.45              |
| 6:F:111:LEU:O   | 6:F:113:GLY:N    | 2.48                     | 0.45              |
| 1:A:332:LYS:C   | 1:A:334:GLY:H    | 2.25                     | 0.45              |
| 1:A:596:THR:C   | 1:A:598:LEU:N    | 2.74                     | 0.45              |
| 1:A:874:ASP:O   | 1:A:875:ALA:C    | 2.59                     | 0.45              |
| 1:A:1044:TRP:O  | 1:A:1045:VAL:C   | 2.59                     | 0.45              |
| 2:B:307:ASP:O   | 2:B:308:TRP:C    | 2.58                     | 0.45              |
| 2:B:492:LEU:O   | 2:B:493:SER:C    | 2.59                     | 0.45              |
| 11:K:40:HIS:O   | 11:K:41:THR:C    | 2.59                     | 0.45              |
| 1:A:17:VAL:HA   | 2:B:1215:ARG:O   | 2.15                     | 0.45              |
| 1:A:250:ILE:O   | 1:A:258:GLY:HA3  | 2.16                     | 0.45              |
| 1:A:289:ILE:O   | 1:A:291:GLU:N    | 2.50                     | 0.45              |
| 1:A:399:HIS:O   | 1:A:400:PRO:C    | 2.58                     | 0.45              |
| 1:A:809:THR:O   | 1:A:810:PRO:C    | 2.59                     | 0.45              |
| 2:B:123:THR:O   | 2:B:125:SER:N    | 2.47                     | 0.45              |
| 2:B:168:GLY:N   | 2:B:450:ALA:HB1  | 2.19                     | 0.45              |
| 2:B:838:SER:CB  | 2:B:989:THR:O    | 2.64                     | 0.45              |
| 5:E:161:LYS:O   | 5:E:163:GLU:N    | 2.49                     | 0.45              |
| 8:H:25:ARG:HA   | 8:H:41:ASP:HA    | 1.98                     | 0.45              |
| 1:A:116:ASP:C   | 1:A:118:HIS:N    | 2.71                     | 0.45              |
| 1:A:512:VAL:C   | 1:A:1067:LEU:CB  | 2.89                     | 0.45              |
| 1:A:618:GLU:O   | 1:A:619:LYS:C    | 2.60                     | 0.45              |
| 1:A:635:ARG:H   | 1:A:877:HIS:N    | 2.00                     | 0.45              |
| 1:A:853:ASP:O   | 1:A:854:ASN:CB   | 2.64                     | 0.45              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1019:CYS:O  | 1:A:1023:ARG:N   | 2.45                     | 0.45              |
| 1:A:1125:ARG:C  | 1:A:1127:ALA:H   | 2.24                     | 0.45              |
| 2:B:435:THR:C   | 2:B:437:GLU:H    | 2.23                     | 0.45              |
| 2:B:654:ARG:O   | 2:B:656:GLY:N    | 2.48                     | 0.45              |
| 3:C:92:CYS:C    | 3:C:94:LYS:N     | 2.72                     | 0.45              |
| 6:F:76:LYS:O    | 7:G:20:PRO:O     | 2.30                     | 0.45              |
| 1:A:509:LEU:CB  | 1:A:1062:GLU:CB  | 2.88                     | 0.45              |
| 1:A:779:PHE:O   | 1:A:780:VAL:C    | 2.59                     | 0.45              |
| 1:A:1019:CYS:O  | 1:A:1020:CYS:C   | 2.60                     | 0.45              |
| 1:A:1349:TYR:O  | 1:A:1350:LYS:C   | 2.60                     | 0.45              |
| 2:B:307:ASP:O   | 2:B:309:GLN:N    | 2.50                     | 0.45              |
| 2:B:410:GLY:O   | 2:B:412:LEU:N    | 2.50                     | 0.45              |
| 1:A:1265:ASN:C  | 1:A:1267:MET:H   | 2.23                     | 0.45              |
| 1:A:1265:ASN:O  | 1:A:1267:MET:N   | 2.50                     | 0.45              |
| 2:B:948:ILE:C   | 2:B:949:VAL:O    | 2.56                     | 0.45              |
| 10:J:34:THR:O   | 10:J:35:ALA:C    | 2.59                     | 0.45              |
| 12:L:38:LEU:O   | 12:L:39:SER:CB   | 2.63                     | 0.45              |
| 12:L:62:LYS:O   | 12:L:63:ARG:C    | 2.59                     | 0.45              |
| 1:A:10:PRO:HA   | 7:G:15:PRO:CB    | 2.46                     | 0.45              |
| 1:A:603:ASN:O   | 1:A:604:GLY:C    | 2.60                     | 0.45              |
| 1:A:1265:ASN:O  | 1:A:1268:LEU:N   | 2.41                     | 0.45              |
| 1:A:1313:LEU:C  | 1:A:1315:GLU:H   | 2.24                     | 0.45              |
| 2:B:641:GLU:C   | 2:B:643:ASP:H    | 2.25                     | 0.45              |
| 2:B:906:SER:O   | 2:B:907:GLY:O    | 2.34                     | 0.45              |
| 5:E:114:ASN:O   | 5:E:115:ASN:CB   | 2.65                     | 0.45              |
| 7:G:50:ASP:O    | 7:G:51:TYR:C     | 2.58                     | 0.45              |
| 1:A:1420:ASP:CB | 5:E:174:GLN:CB   | 2.95                     | 0.45              |
| 2:B:1137:CYS:O  | 2:B:1140:ALA:HB3 | 2.17                     | 0.45              |
| 1:A:236:LEU:N   | 4:D:16:LYS:N     | 2.60                     | 0.45              |
| 1:A:236:LEU:O   | 4:D:16:LYS:CA    | 2.56                     | 0.45              |
| 1:A:270:LEU:O   | 1:A:271:LYS:C    | 2.60                     | 0.45              |
| 1:A:384:ASN:HA  | 6:F:105:ALA:HB2  | 1.99                     | 0.45              |
| 2:B:114:PRO:O   | 2:B:117:ALA:N    | 2.48                     | 0.45              |
| 2:B:769:TYR:O   | 2:B:772:ALA:N    | 2.50                     | 0.45              |
| 2:B:769:TYR:C   | 2:B:771:SER:N    | 2.73                     | 0.45              |
| 2:B:1034:VAL:C  | 2:B:1036:ALA:N   | 2.72                     | 0.45              |
| 2:B:1220:ARG:CB | 6:F:139:PRO:CB   | 2.95                     | 0.45              |
| 1:A:71:GLN:O    | 1:A:73:GLY:N     | 2.38                     | 0.45              |
| 1:A:498:ARG:O   | 1:A:501:LEU:N    | 2.47                     | 0.45              |
| 1:A:767:GLN:HA  | 1:A:815:PHE:O    | 2.17                     | 0.45              |
| 1:A:776:ALA:HB1 | 2:B:397:ASP:CB   | 2.47                     | 0.45              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:859:SER:CA  | 1:A:1437:GLY:N   | 2.80                     | 0.45              |
| 1:A:1011:GLN:O  | 1:A:1012:ARG:C   | 2.60                     | 0.45              |
| 1:A:1213:GLY:O  | 1:A:1214:GLU:C   | 2.59                     | 0.45              |
| 2:B:882:THR:O   | 2:B:883:LEU:CB   | 2.65                     | 0.45              |
| 2:B:1192:TYR:CA | 7:G:67:SER:C     | 2.85                     | 0.45              |
| 5:E:16:PHE:O    | 5:E:17:ARG:C     | 2.59                     | 0.45              |
| 8:H:11:GLN:O    | 8:H:28:ALA:HB1   | 2.17                     | 0.45              |
| 11:K:87:LEU:O   | 11:K:88:LYS:C    | 2.60                     | 0.45              |
| 1:A:103:CYS:O   | 1:A:106:VAL:O    | 2.35                     | 0.44              |
| 1:A:1388:GLY:C  | 1:A:1390:ASN:H   | 2.25                     | 0.44              |
| 2:B:265:SER:O   | 2:B:266:ALA:CB   | 2.65                     | 0.44              |
| 2:B:418:LYS:C   | 2:B:420:LEU:N    | 2.75                     | 0.44              |
| 2:B:1197:PRO:O  | 2:B:1200:ALA:N   | 2.48                     | 0.44              |
| 1:A:909:ASP:C   | 1:A:911:SER:H    | 2.25                     | 0.44              |
| 1:A:1015:VAL:O  | 1:A:1018:PHE:N   | 2.49                     | 0.44              |
| 1:A:1343:ALA:O  | 1:A:1346:ALA:HB3 | 2.16                     | 0.44              |
| 2:B:258:LEU:O   | 2:B:259:TYR:O    | 2.35                     | 0.44              |
| 2:B:593:PRO:O   | 2:B:594:ALA:C    | 2.60                     | 0.44              |
| 5:E:147:HIS:O   | 5:E:148:GLU:C    | 2.61                     | 0.44              |
| 10:J:56:LEU:O   | 10:J:57:ILE:C    | 2.58                     | 0.44              |
| 1:A:344:ARG:C   | 2:B:1130:PHE:N   | 2.75                     | 0.44              |
| 1:A:418:SER:C   | 1:A:420:ARG:H    | 2.24                     | 0.44              |
| 1:A:514:PRO:C   | 1:A:1367:HIS:HA  | 2.42                     | 0.44              |
| 1:A:528:LEU:O   | 1:A:529:CYS:C    | 2.60                     | 0.44              |
| 1:A:860:LEU:CB  | 1:A:1422:ARG:H   | 2.30                     | 0.44              |
| 1:A:1364:ASN:O  | 1:A:1365:TYR:C   | 2.50                     | 0.44              |
| 1:A:1393:ASN:O  | 1:A:1397:LEU:CB  | 2.52                     | 0.44              |
| 2:B:769:TYR:C   | 2:B:771:SER:H    | 2.26                     | 0.44              |
| 3:C:83:SER:O    | 3:C:85:ASP:N     | 2.51                     | 0.44              |
| 1:A:3:GLY:O     | 1:A:377:PRO:O    | 2.10                     | 0.44              |
| 1:A:334:GLY:O   | 1:A:335:ARG:C    | 2.60                     | 0.44              |
| 1:A:766:GLY:N   | 1:A:816:HIS:CA   | 2.51                     | 0.44              |
| 1:A:1053:PHE:O  | 1:A:1055:ARG:N   | 2.50                     | 0.44              |
| 1:A:1142:THR:O  | 1:A:1143:LEU:C   | 2.61                     | 0.44              |
| 2:B:410:GLY:O   | 2:B:411:PRO:C    | 2.61                     | 0.44              |
| 2:B:581:PHE:HA  | 2:B:585:VAL:O    | 2.17                     | 0.44              |
| 3:C:27:LEU:O    | 3:C:30:ALA:N     | 2.50                     | 0.44              |
| 10:J:28:ASP:O   | 10:J:29:GLU:C    | 2.61                     | 0.44              |
| 11:K:53:ASP:O   | 11:K:55:LYS:N    | 2.50                     | 0.44              |
| 1:A:206:GLU:O   | 1:A:207:ILE:C    | 2.60                     | 0.44              |
| 1:A:1122:LYS:O  | 1:A:1125:ARG:N   | 2.51                     | 0.44              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:B:45:SER:O    | 2:B:46:GLN:C    | 2.60                     | 0.44              |
| 5:E:98:ILE:O    | 5:E:99:HIS:C    | 2.59                     | 0.44              |
| 6:F:73:ALA:H    | 7:G:69:GLU:C    | 2.08                     | 0.44              |
| 1:A:296:LEU:O   | 1:A:297:GLN:C   | 2.59                     | 0.44              |
| 1:A:452:LYS:CB  | 1:A:846:GLU:CA  | 2.85                     | 0.44              |
| 1:A:645:LEU:O   | 1:A:646:PHE:C   | 2.59                     | 0.44              |
| 2:B:604:ARG:C   | 2:B:606:LYS:H   | 2.26                     | 0.44              |
| 3:C:105:GLY:HA3 | 3:C:149:LYS:O   | 2.17                     | 0.44              |
| 6:F:143:PHE:CB  | 7:G:68:ALA:HB2  | 0.92                     | 0.44              |
| 1:A:765:VAL:C   | 1:A:820:GLY:HA3 | 2.43                     | 0.44              |
| 1:A:1119:GLU:O  | 1:A:1120:GLN:C  | 2.61                     | 0.44              |
| 2:B:1177:HIS:O  | 2:B:1179:GLN:N  | 2.50                     | 0.44              |
| 10:J:8:PHE:O    | 10:J:9:SER:C    | 2.60                     | 0.44              |
| 1:A:862:ASN:C   | 1:A:1422:ARG:CB | 2.91                     | 0.44              |
| 1:A:901:LEU:O   | 1:A:921:GLY:N   | 2.48                     | 0.44              |
| 1:A:1448:GLU:C  | 7:G:27:LYS:O    | 2.61                     | 0.44              |
| 2:B:1145:SER:CB | 2:B:1195:HIS:N  | 2.81                     | 0.44              |
| 1:A:62:ASP:O    | 1:A:63:ARG:C    | 2.61                     | 0.44              |
| 1:A:73:GLY:O    | 1:A:74:MET:C    | 2.61                     | 0.44              |
| 1:A:418:SER:C   | 1:A:420:ARG:N   | 2.75                     | 0.44              |
| 1:A:1205:LYS:O  | 1:A:1206:ASP:C  | 2.59                     | 0.44              |
| 2:B:312:GLU:CA  | 9:I:46:HIS:CB   | 2.84                     | 0.44              |
| 6:F:138:LEU:H   | 7:G:60:ARG:C    | 2.26                     | 0.44              |
| 9:I:3:THR:H     | 9:I:45:ARG:CB   | 2.30                     | 0.44              |
| 10:J:1:MET:H2   | 10:J:55:ASP:C   | 2.26                     | 0.44              |
| 11:K:53:ASP:C   | 11:K:55:LYS:N   | 2.76                     | 0.44              |
| 1:A:2:VAL:HA    | 1:A:492:PRO:O   | 2.10                     | 0.43              |
| 1:A:51:GLY:HA2  | 1:A:56:PRO:HA   | 2.00                     | 0.43              |
| 1:A:282:ASN:O   | 1:A:284:ALA:N   | 2.51                     | 0.43              |
| 2:B:460:ALA:C   | 2:B:462:ALA:H   | 2.26                     | 0.43              |
| 3:C:163:ILE:C   | 3:C:165:LYS:H   | 2.25                     | 0.43              |
| 10:J:16:ASP:C   | 10:J:18:TRP:H   | 2.26                     | 0.43              |
| 12:L:58:LYS:O   | 12:L:59:ALA:O   | 2.34                     | 0.43              |
| 1:A:9:ALA:HB1   | 7:G:67:SER:CB   | 2.48                     | 0.43              |
| 1:A:95:PHE:O    | 1:A:98:LYS:N    | 2.49                     | 0.43              |
| 2:B:418:LYS:O   | 2:B:420:LEU:N   | 2.51                     | 0.43              |
| 2:B:619:ILE:O   | 2:B:622:LYS:N   | 2.50                     | 0.43              |
| 8:H:82:PRO:C    | 8:H:84:ALA:N    | 2.75                     | 0.43              |
| 1:A:874:ASP:O   | 1:A:876:ALA:N   | 2.50                     | 0.43              |
| 1:A:1208:THR:O  | 1:A:1209:MET:C  | 2.62                     | 0.43              |
| 1:A:1315:GLU:C  | 1:A:1317:MET:N  | 2.75                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:B:386:LEU:O   | 2:B:387:LEU:C    | 2.61                     | 0.43              |
| 2:B:765:PRO:O   | 2:B:767:ASN:N    | 2.51                     | 0.43              |
| 2:B:806:THR:C   | 2:B:808:ALA:N    | 2.76                     | 0.43              |
| 3:C:256:ALA:C   | 3:C:258:ILE:N    | 2.77                     | 0.43              |
| 1:A:244:PRO:O   | 1:A:245:PRO:C    | 2.61                     | 0.43              |
| 1:A:515:GLN:C   | 1:A:1367:HIS:O   | 2.61                     | 0.43              |
| 1:A:659:HIS:C   | 1:A:661:GLY:H    | 2.26                     | 0.43              |
| 1:A:1409:LEU:O  | 1:A:1412:ALA:HB3 | 2.17                     | 0.43              |
| 3:C:245:VAL:C   | 3:C:247:GLY:N    | 2.74                     | 0.43              |
| 6:F:135:ARG:CB  | 7:G:15:PRO:CB    | 2.95                     | 0.43              |
| 8:H:11:GLN:HA   | 8:H:53:ASP:O     | 2.18                     | 0.43              |
| 1:A:1105:SER:O  | 1:A:1106:LEU:CB  | 2.67                     | 0.43              |
| 1:A:1444:MET:C  | 6:F:72:LYS:C     | 2.84                     | 0.43              |
| 2:B:20:ASP:C    | 2:B:22:SER:H     | 2.27                     | 0.43              |
| 2:B:388:CYS:HA  | 9:I:92:ARG:HA    | 2.00                     | 0.43              |
| 2:B:435:THR:C   | 2:B:437:GLU:N    | 2.74                     | 0.43              |
| 2:B:595:ARG:O   | 2:B:596:LEU:C    | 2.59                     | 0.43              |
| 2:B:730:ARG:O   | 2:B:731:VAL:O    | 2.36                     | 0.43              |
| 1:A:800:VAL:H   | 1:A:817:ALA:C    | 2.23                     | 0.43              |
| 1:A:1425:SER:O  | 1:A:1426:GLU:C   | 2.61                     | 0.43              |
| 2:B:263:GLY:O   | 2:B:264:SER:C    | 2.62                     | 0.43              |
| 2:B:394:ASP:N   | 9:I:92:ARG:O     | 2.51                     | 0.43              |
| 3:C:92:CYS:O    | 3:C:94:LYS:N     | 2.52                     | 0.43              |
| 5:E:191:LYS:O   | 5:E:192:ARG:C    | 2.62                     | 0.43              |
| 1:A:387:ARG:HA  | 6:F:104:ASN:CB   | 2.48                     | 0.43              |
| 1:A:858:ASN:CA  | 1:A:1422:ARG:CA  | 2.61                     | 0.43              |
| 1:A:1427:ASN:CA | 2:B:1138:MET:O   | 2.64                     | 0.43              |
| 1:A:1444:MET:C  | 2:B:1190:ASP:O   | 2.60                     | 0.43              |
| 4:D:138:ASN:O   | 4:D:140:ASP:N    | 2.52                     | 0.43              |
| 10:J:32:GLU:O   | 10:J:33:GLY:C    | 2.62                     | 0.43              |
| 1:A:450:LEU:HA  | 1:A:843:LYS:CB   | 2.49                     | 0.43              |
| 1:A:503:GLN:O   | 1:A:1061:GLY:C   | 2.62                     | 0.43              |
| 1:A:573:SER:O   | 1:A:574:GLY:C    | 2.61                     | 0.43              |
| 6:F:98:ALA:O    | 6:F:99:LEU:C     | 2.62                     | 0.43              |
| 11:K:96:ASN:O   | 11:K:97:LYS:C    | 2.62                     | 0.43              |
| 1:A:67:CYS:O    | 1:A:68:GLN:CB    | 2.67                     | 0.43              |
| 1:A:73:GLY:O    | 1:A:75:ASN:N     | 2.52                     | 0.43              |
| 1:A:513:SER:N   | 1:A:1067:LEU:CB  | 2.82                     | 0.43              |
| 1:A:807:GLY:HA2 | 2:B:760:ASP:O    | 2.19                     | 0.43              |
| 1:A:839:ARG:O   | 1:A:840:ARG:C    | 2.60                     | 0.43              |
| 1:A:1209:MET:O  | 1:A:1210:GLY:C   | 2.61                     | 0.43              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:B:281:PRO:C   | 2:B:283:VAL:N    | 2.76                     | 0.43              |
| 2:B:432:MET:C   | 2:B:434:ARG:H    | 2.26                     | 0.43              |
| 2:B:446:LEU:O   | 2:B:447:ALA:CB   | 2.66                     | 0.43              |
| 2:B:582:VAL:HA  | 2:B:626:ILE:O    | 2.19                     | 0.43              |
| 2:B:1032:SER:O  | 2:B:1036:ALA:HB2 | 2.19                     | 0.43              |
| 6:F:72:LYS:HA   | 7:G:10:ASN:HA    | 2.00                     | 0.43              |
| 6:F:77:ASP:N    | 7:G:23:LYS:CA    | 2.72                     | 0.43              |
| 11:K:53:ASP:C   | 11:K:55:LYS:H    | 2.26                     | 0.43              |
| 1:A:574:GLY:O   | 1:A:575:LYS:C    | 2.62                     | 0.43              |
| 1:A:1409:LEU:O  | 1:A:1410:PHE:C   | 2.62                     | 0.43              |
| 2:B:31:TRP:O    | 2:B:32:ALA:C     | 2.62                     | 0.43              |
| 2:B:377:PHE:C   | 2:B:379:GLY:H    | 2.27                     | 0.43              |
| 2:B:593:PRO:O   | 2:B:596:LEU:N    | 2.52                     | 0.43              |
| 3:C:92:CYS:C    | 3:C:94:LYS:H     | 2.27                     | 0.43              |
| 4:D:29:LEU:O    | 4:D:30:GLY:C     | 2.62                     | 0.43              |
| 1:A:1121:ALA:O  | 1:A:1122:LYS:C   | 2.62                     | 0.42              |
| 2:B:765:PRO:C   | 2:B:767:ASN:N    | 2.77                     | 0.42              |
| 6:F:138:LEU:N   | 7:G:61:ILE:N     | 2.66                     | 0.42              |
| 1:A:231:PRO:O   | 1:A:233:TRP:N    | 2.52                     | 0.42              |
| 1:A:432:VAL:O   | 1:A:433:GLU:C    | 2.60                     | 0.42              |
| 1:A:608:ILE:C   | 1:A:610:GLY:N    | 2.72                     | 0.42              |
| 1:A:778:GLY:C   | 2:B:402:GLY:N    | 2.73                     | 0.42              |
| 2:B:644:GLU:C   | 2:B:646:LEU:N    | 2.77                     | 0.42              |
| 2:B:1029:CYS:HA | 2:B:1089:PRO:O   | 2.19                     | 0.42              |
| 4:D:53:SER:CB   | 4:D:153:ARG:H    | 2.32                     | 0.42              |
| 9:I:3:THR:N     | 9:I:45:ARG:CB    | 2.82                     | 0.42              |
| 1:A:226:GLU:CB  | 4:D:9:GLN:CB     | 2.97                     | 0.42              |
| 1:A:241:VAL:O   | 1:A:242:PRO:C    | 2.61                     | 0.42              |
| 1:A:660:ASN:O   | 1:A:661:GLY:O    | 2.37                     | 0.42              |
| 1:A:679:ILE:O   | 1:A:682:THR:N    | 2.52                     | 0.42              |
| 1:A:809:THR:C   | 2:B:729:ILE:CB   | 2.92                     | 0.42              |
| 1:A:890:ASP:H   | 1:A:1296:GLY:HA3 | 1.84                     | 0.42              |
| 1:A:1447:GLU:O  | 7:G:29:LYS:CB    | 2.47                     | 0.42              |
| 1:A:1452:LYS:CA | 7:G:28:THR:CB    | 2.97                     | 0.42              |
| 2:B:257:LYS:N   | 2:B:270:LYS:O    | 2.52                     | 0.42              |
| 2:B:312:GLU:O   | 2:B:315:LYS:N    | 2.50                     | 0.42              |
| 9:I:56:ALA:O    | 9:I:57:GLY:C     | 2.63                     | 0.42              |
| 9:I:61:ASP:C    | 9:I:63:GLY:N     | 2.73                     | 0.42              |
| 1:A:457:ALA:HB3 | 1:A:506:ALA:HA   | 2.01                     | 0.42              |
| 1:A:631:HIS:C   | 1:A:876:ALA:CA   | 2.92                     | 0.42              |
| 1:A:800:VAL:N   | 1:A:815:PHE:O    | 2.50                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:1070:GLN:O  | 1:A:1071:SER:C   | 2.62                     | 0.42              |
| 1:A:1164:PRO:C  | 1:A:1166:ASP:N   | 2.76                     | 0.42              |
| 2:B:394:ASP:HA  | 9:I:92:ARG:O     | 2.20                     | 0.42              |
| 2:B:814:PHE:C   | 2:B:816:GLU:H    | 2.27                     | 0.42              |
| 2:B:986:GLN:O   | 2:B:987:LYS:C    | 2.62                     | 0.42              |
| 2:B:1149:GLU:C  | 2:B:1157:ALA:N   | 2.77                     | 0.42              |
| 6:F:72:LYS:O    | 6:F:73:ALA:HB3   | 2.20                     | 0.42              |
| 1:A:120:GLU:C   | 1:A:122:MET:H    | 2.26                     | 0.42              |
| 1:A:277:GLU:O   | 1:A:279:LEU:N    | 2.52                     | 0.42              |
| 1:A:1340:GLY:O  | 1:A:1341:ILE:C   | 2.62                     | 0.42              |
| 2:B:458:LYS:O   | 2:B:459:TYR:C    | 2.61                     | 0.42              |
| 4:D:206:GLU:O   | 4:D:208:GLU:N    | 2.53                     | 0.42              |
| 2:B:575:PRO:C   | 2:B:577:ALA:H    | 2.26                     | 0.42              |
| 2:B:654:ARG:C   | 2:B:656:GLY:N    | 2.77                     | 0.42              |
| 2:B:957:ASN:O   | 2:B:958:GLN:C    | 2.63                     | 0.42              |
| 2:B:1148:LYS:CA | 2:B:1200:ALA:N   | 2.73                     | 0.42              |
| 4:D:141:LEU:O   | 4:D:142:LYS:C    | 2.61                     | 0.42              |
| 5:E:20:LYS:O    | 5:E:21:GLU:C     | 2.62                     | 0.42              |
| 5:E:127:ILE:O   | 5:E:130:ALA:HB3  | 2.20                     | 0.42              |
| 1:A:100:LYS:O   | 1:A:102:VAL:N    | 2.52                     | 0.42              |
| 1:A:268:ASP:O   | 1:A:269:ILE:C    | 2.62                     | 0.42              |
| 1:A:335:ARG:HA  | 1:A:339:ASN:CB   | 2.50                     | 0.42              |
| 1:A:1313:LEU:C  | 1:A:1315:GLU:N   | 2.78                     | 0.42              |
| 1:A:1428:VAL:CA | 2:B:1138:MET:CB  | 2.75                     | 0.42              |
| 2:B:578:THR:O   | 2:B:579:ARG:C    | 2.62                     | 0.42              |
| 4:D:167:LEU:C   | 4:D:169:SER:H    | 2.28                     | 0.42              |
| 5:E:90:VAL:CA   | 5:E:120:ALA:HB2  | 2.49                     | 0.42              |
| 1:A:29:ALA:HB1  | 2:B:1184:GLY:HA2 | 2.00                     | 0.42              |
| 1:A:42:ASP:C    | 1:A:44:THR:N     | 2.77                     | 0.42              |
| 1:A:341:MET:O   | 2:B:1131:GLY:O   | 2.38                     | 0.42              |
| 1:A:817:ALA:O   | 1:A:820:GLY:N    | 2.53                     | 0.42              |
| 2:B:293:PRO:C   | 2:B:294:ASP:O    | 2.59                     | 0.42              |
| 2:B:366:GLN:O   | 2:B:367:LEU:O    | 2.38                     | 0.42              |
| 2:B:792:MET:HA  | 2:B:856:PHE:O    | 2.20                     | 0.42              |
| 4:D:66:ARG:O    | 4:D:67:ARG:C     | 2.61                     | 0.42              |
| 6:F:77:ASP:CA   | 7:G:21:ARG:HA    | 2.48                     | 0.42              |
| 7:G:149:GLY:O   | 7:G:159:ALA:HB1  | 2.20                     | 0.42              |
| 8:H:89:LEU:C    | 8:H:91:ASP:N     | 2.68                     | 0.42              |
| 11:K:17:SER:O   | 11:K:18:LYS:C    | 2.62                     | 0.42              |
| 1:A:472:LEU:O   | 1:A:475:THR:CB   | 2.68                     | 0.42              |
| 1:A:1217:LYS:O  | 1:A:1221:LYS:N   | 2.52                     | 0.42              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:B:460:ALA:C   | 2:B:462:ALA:N   | 2.76                     | 0.42              |
| 2:B:610:ASN:O   | 2:B:612:GLU:N   | 2.53                     | 0.42              |
| 2:B:610:ASN:C   | 2:B:612:GLU:H   | 2.28                     | 0.42              |
| 2:B:681:TRP:C   | 2:B:683:SER:N   | 2.78                     | 0.42              |
| 2:B:1182:CYS:O  | 2:B:1183:LYS:O  | 2.37                     | 0.42              |
| 3:C:247:GLY:C   | 3:C:249:ASP:N   | 2.77                     | 0.42              |
| 1:A:77:CYS:C    | 1:A:78:PRO:O    | 2.45                     | 0.42              |
| 1:A:148:CYS:O   | 1:A:168:GLY:HA2 | 2.19                     | 0.42              |
| 1:A:845:LEU:O   | 1:A:1434:ALA:O  | 2.38                     | 0.42              |
| 1:A:1376:THR:O  | 1:A:1377:THR:C  | 2.62                     | 0.42              |
| 1:A:1449:SER:CA | 7:G:28:THR:N    | 2.77                     | 0.42              |
| 2:B:593:PRO:O   | 2:B:595:ARG:N   | 2.53                     | 0.42              |
| 2:B:844:SER:O   | 2:B:845:SER:C   | 2.62                     | 0.42              |
| 2:B:1208:MET:HA | 2:B:1212:ILE:O  | 2.20                     | 0.42              |
| 3:C:62:PHE:O    | 3:C:63:ILE:C    | 2.61                     | 0.42              |
| 3:C:226:ASP:O   | 3:C:227:THR:CB  | 2.66                     | 0.42              |
| 4:D:144:THR:O   | 4:D:148:LEU:CB  | 2.68                     | 0.42              |
| 1:A:209:ASN:O   | 1:A:210:ILE:C   | 2.62                     | 0.41              |
| 1:A:525:GLN:O   | 1:A:526:ASP:C   | 2.63                     | 0.41              |
| 1:A:1157:ASP:O  | 1:A:1159:ARG:N  | 2.53                     | 0.41              |
| 2:B:644:GLU:C   | 2:B:646:LEU:H   | 2.28                     | 0.41              |
| 2:B:1149:GLU:CB | 2:B:1158:PHE:CB | 2.98                     | 0.41              |
| 4:D:217:LEU:O   | 4:D:219:THR:N   | 2.53                     | 0.41              |
| 6:F:72:LYS:HA   | 7:G:11:ILE:H    | 1.85                     | 0.41              |
| 7:G:123:ALA:C   | 7:G:125:SER:H   | 2.28                     | 0.41              |
| 1:A:57:ARG:C    | 1:A:58:LEU:O    | 2.62                     | 0.41              |
| 1:A:203:SER:O   | 1:A:204:THR:C   | 2.62                     | 0.41              |
| 1:A:630:ILE:O   | 1:A:631:HIS:C   | 2.63                     | 0.41              |
| 1:A:738:LYS:C   | 1:A:740:LEU:N   | 2.78                     | 0.41              |
| 1:A:825:ILE:O   | 1:A:826:ASP:C   | 2.62                     | 0.41              |
| 5:E:117:THR:C   | 5:E:119:SER:H   | 2.27                     | 0.41              |
| 1:A:1115:ALA:C  | 1:A:1117:ASP:H  | 2.29                     | 0.41              |
| 1:A:1157:ASP:C  | 1:A:1159:ARG:N  | 2.77                     | 0.41              |
| 2:B:1124:ARG:O  | 2:B:1125:ASP:CB | 2.68                     | 0.41              |
| 3:C:9:LYS:O     | 3:C:10:ILE:C    | 2.63                     | 0.41              |
| 3:C:174:ALA:O   | 3:C:175:ALA:CB  | 2.67                     | 0.41              |
| 5:E:43:LYS:O    | 5:E:45:LYS:N    | 2.48                     | 0.41              |
| 5:E:98:ILE:O    | 5:E:100:ILE:N   | 2.54                     | 0.41              |
| 5:E:117:THR:O   | 5:E:120:ALA:N   | 2.44                     | 0.41              |
| 5:E:201:LYS:HA  | 5:E:206:GLY:O   | 2.19                     | 0.41              |
| 10:J:52:THR:O   | 10:J:53:HIS:C   | 2.63                     | 0.41              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:264:PHE:O   | 1:A:267:ALA:HB3 | 2.20                     | 0.41              |
| 1:A:514:PRO:C   | 1:A:516:SER:N   | 2.75                     | 0.41              |
| 1:A:1406:VAL:O  | 1:A:1407:GLU:C  | 2.63                     | 0.41              |
| 2:B:29:ASP:O    | 2:B:30:SER:C    | 2.64                     | 0.41              |
| 2:B:314:LEU:O   | 2:B:315:LYS:C   | 2.62                     | 0.41              |
| 2:B:388:CYS:C   | 2:B:390:LEU:H   | 2.28                     | 0.41              |
| 2:B:1146:PHE:CA | 2:B:1196:ILE:C  | 2.91                     | 0.41              |
| 9:I:83:ASN:HA   | 9:I:102:VAL:O   | 2.20                     | 0.41              |
| 1:A:332:LYS:C   | 1:A:334:GLY:N   | 2.78                     | 0.41              |
| 1:A:744:LYS:O   | 1:A:747:VAL:N   | 2.54                     | 0.41              |
| 2:B:737:THR:O   | 2:B:738:PHE:C   | 2.62                     | 0.41              |
| 2:B:1200:ALA:O  | 2:B:1201:LYS:C  | 2.63                     | 0.41              |
| 6:F:95:GLY:O    | 6:F:96:THR:C    | 2.64                     | 0.41              |
| 6:F:138:LEU:CA  | 7:G:59:GLY:O    | 2.61                     | 0.41              |
| 7:G:166:ASP:C   | 7:G:168:LEU:N   | 2.79                     | 0.41              |
| 8:H:56:THR:O    | 8:H:144:ILE:HA  | 2.21                     | 0.41              |
| 9:I:88:SER:C    | 9:I:90:GLN:H    | 2.29                     | 0.41              |
| 1:A:836:TYR:O   | 1:A:837:ILE:C   | 2.63                     | 0.41              |
| 1:A:909:ASP:C   | 1:A:911:SER:N   | 2.79                     | 0.41              |
| 2:B:214:ALA:HB3 | 2:B:498:THR:HA  | 2.01                     | 0.41              |
| 2:B:552:MET:O   | 2:B:554:ILE:N   | 2.53                     | 0.41              |
| 2:B:814:PHE:C   | 2:B:816:GLU:N   | 2.77                     | 0.41              |
| 4:D:62:ALA:C    | 4:D:64:VAL:N    | 2.78                     | 0.41              |
| 1:A:98:LYS:C    | 1:A:100:LYS:N   | 2.77                     | 0.41              |
| 1:A:220:THR:O   | 1:A:221:SER:C   | 2.64                     | 0.41              |
| 1:A:343:LYS:O   | 2:B:1129:ARG:CB | 2.65                     | 0.41              |
| 1:A:482:PHE:C   | 1:A:484:GLY:N   | 2.77                     | 0.41              |
| 1:A:800:VAL:C   | 1:A:814:PHE:C   | 2.71                     | 0.41              |
| 1:A:1396:ALA:O  | 1:A:1397:LEU:C  | 2.64                     | 0.41              |
| 1:A:1420:ASP:CB | 5:E:174:GLN:HA  | 2.50                     | 0.41              |
| 2:B:34:ILE:O    | 2:B:35:SER:C    | 2.63                     | 0.41              |
| 2:B:1064:TYR:O  | 2:B:1065:GLN:C  | 2.63                     | 0.41              |
| 4:D:40:HIS:C    | 4:D:42:GLY:N    | 2.78                     | 0.41              |
| 4:D:128:VAL:O   | 4:D:129:LEU:C   | 2.64                     | 0.41              |
| 6:F:143:PHE:CA  | 7:G:68:ALA:HB3  | 1.96                     | 0.41              |
| 1:A:226:GLU:CB  | 4:D:9:GLN:HA    | 2.50                     | 0.41              |
| 1:A:276:LEU:O   | 1:A:279:LEU:N   | 2.47                     | 0.41              |
| 1:A:473:SER:C   | 1:A:475:THR:H   | 2.27                     | 0.41              |
| 1:A:526:ASP:O   | 1:A:527:THR:C   | 2.63                     | 0.41              |
| 1:A:859:SER:HA  | 1:A:1437:GLY:N  | 2.36                     | 0.41              |
| 1:A:1056:SER:C  | 1:A:1057:VAL:O  | 2.63                     | 0.41              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:B:410:GLY:C   | 2:B:412:LEU:N    | 2.79                     | 0.41              |
| 2:B:597:MET:C   | 2:B:599:THR:N    | 2.79                     | 0.41              |
| 2:B:763:GLN:O   | 2:B:764:SER:C    | 2.64                     | 0.41              |
| 2:B:1192:TYR:CB | 7:G:67:SER:C     | 2.92                     | 0.41              |
| 3:C:26:ASP:O    | 3:C:27:LEU:C     | 2.64                     | 0.41              |
| 5:E:181:ALA:O   | 5:E:182:ASP:C    | 2.64                     | 0.41              |
| 1:A:14:VAL:CB   | 2:B:1144:ALA:HB3 | 2.50                     | 0.41              |
| 1:A:532:ARG:O   | 1:A:533:LYS:C    | 2.64                     | 0.41              |
| 1:A:566:ILE:O   | 1:A:567:LYS:O    | 2.39                     | 0.41              |
| 1:A:635:ARG:CB  | 1:A:874:ASP:N    | 2.84                     | 0.41              |
| 1:A:695:LYS:C   | 1:A:697:ALA:N    | 2.79                     | 0.41              |
| 1:A:697:ALA:C   | 1:A:699:ALA:H    | 2.29                     | 0.41              |
| 1:A:801:GLU:CA  | 1:A:816:HIS:CB   | 2.98                     | 0.41              |
| 1:A:940:ARG:O   | 1:A:941:LYS:C    | 2.62                     | 0.41              |
| 1:A:1048:ASN:O  | 1:A:1049:ILE:C   | 2.64                     | 0.41              |
| 1:A:1332:PHE:O  | 1:A:1333:ILE:C   | 2.64                     | 0.41              |
| 1:A:1388:GLY:C  | 1:A:1390:ASN:N   | 2.79                     | 0.41              |
| 2:B:294:ASP:C   | 2:B:296:GLU:H    | 2.29                     | 0.41              |
| 2:B:511:PRO:O   | 2:B:513:GLN:N    | 2.54                     | 0.41              |
| 2:B:1068:GLY:C  | 2:B:1069:PHE:O   | 2.64                     | 0.41              |
| 4:D:52:LEU:C    | 4:D:54:GLU:H     | 2.29                     | 0.41              |
| 4:D:128:VAL:C   | 4:D:130:LEU:N    | 2.78                     | 0.41              |
| 11:K:52:ASN:O   | 11:K:53:ASP:C    | 2.64                     | 0.41              |
| 1:A:482:PHE:O   | 1:A:484:GLY:N    | 2.53                     | 0.41              |
| 1:A:625:SER:C   | 1:A:1362:TYR:O   | 2.63                     | 0.41              |
| 1:A:794:PRO:C   | 1:A:796:SER:N    | 2.78                     | 0.41              |
| 1:A:1164:PRO:C  | 1:A:1166:ASP:H   | 2.28                     | 0.41              |
| 1:A:1242:VAL:O  | 1:A:1243:VAL:CB  | 2.69                     | 0.41              |
| 2:B:838:SER:CA  | 2:B:989:THR:O    | 2.69                     | 0.41              |
| 2:B:1185:CYS:N  | 4:D:4:SER:N      | 2.63                     | 0.41              |
| 3:C:168:ALA:O   | 3:C:169:LYS:C    | 2.64                     | 0.41              |
| 8:H:106:GLU:O   | 8:H:108:SER:N    | 2.48                     | 0.41              |
| 1:A:274:ILE:O   | 1:A:275:SER:C    | 2.62                     | 0.40              |
| 1:A:589:GLN:N   | 1:A:880:LYS:O    | 2.53                     | 0.40              |
| 1:A:1074:GLU:C  | 1:A:1076:ALA:H   | 2.27                     | 0.40              |
| 3:C:59:ALA:O    | 3:C:60:ASP:C     | 2.64                     | 0.40              |
| 5:E:9:ILE:C     | 5:E:11:ARG:N     | 2.78                     | 0.40              |
| 1:A:23:SER:C    | 1:A:25:GLU:N     | 2.78                     | 0.40              |
| 1:A:1438:THR:CB | 2:B:1144:ALA:HB3 | 2.51                     | 0.40              |
| 2:B:189:LEU:O   | 2:B:190:TYR:C    | 2.61                     | 0.40              |
| 2:B:294:ASP:O   | 2:B:296:GLU:N    | 2.48                     | 0.40              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 2:B:312:GLU:O  | 2:B:313:MET:C   | 2.62                     | 0.40              |
| 3:C:163:ILE:C  | 3:C:165:LYS:N   | 2.79                     | 0.40              |
| 7:G:111:THR:O  | 7:G:112:LYS:C   | 2.64                     | 0.40              |
| 1:A:451:HIS:O  | 1:A:452:LYS:C   | 2.63                     | 0.40              |
| 1:A:516:SER:O  | 1:A:517:ASN:C   | 2.64                     | 0.40              |
| 1:A:626:ASN:HA | 1:A:1363:VAL:C  | 2.46                     | 0.40              |
| 1:A:823:GLY:O  | 1:A:824:LEU:C   | 2.64                     | 0.40              |
| 1:A:1442:ASP:O | 6:F:141:GLY:HA3 | 2.20                     | 0.40              |
| 2:B:392:ARG:HA | 9:I:90:GLN:CB   | 2.47                     | 0.40              |
| 2:B:759:PRO:C  | 2:B:761:HIS:H   | 2.29                     | 0.40              |
| 2:B:841:MET:O  | 2:B:993:THR:HA  | 2.21                     | 0.40              |
| 3:C:208:GLU:C  | 3:C:210:GLU:N   | 2.80                     | 0.40              |
| 8:H:96:VAL:HA  | 8:H:142:LEU:O   | 2.21                     | 0.40              |
| 1:A:23:SER:O   | 1:A:25:GLU:N    | 2.55                     | 0.40              |
| 1:A:103:CYS:C  | 1:A:105:CYS:N   | 2.78                     | 0.40              |
| 2:B:1135:ARG:O | 2:B:1138:MET:N  | 2.54                     | 0.40              |
| 3:C:18:VAL:O   | 3:C:19:ASP:C    | 2.64                     | 0.40              |
| 4:D:138:ASN:O  | 4:D:141:LEU:N   | 2.54                     | 0.40              |
| 5:E:42:PHE:O   | 5:E:43:LYS:C    | 2.65                     | 0.40              |
| 1:A:296:LEU:C  | 1:A:298:PHE:N   | 2.78                     | 0.40              |
| 1:A:653:VAL:O  | 1:A:654:ASN:C   | 2.64                     | 0.40              |
| 1:A:659:HIS:C  | 1:A:661:GLY:N   | 2.79                     | 0.40              |
| 1:A:683:ILE:O  | 1:A:686:ALA:HB3 | 2.21                     | 0.40              |
| 1:A:1001:ARG:O | 1:A:1002:GLY:C  | 2.64                     | 0.40              |
| 2:B:1027:ILE:O | 2:B:1028:GLU:C  | 2.64                     | 0.40              |
| 5:E:39:LEU:O   | 5:E:40:GLU:C    | 2.64                     | 0.40              |
| 11:K:83:PRO:O  | 11:K:84:LYS:C   | 2.64                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-----------|-------------|----|
| 1   | A     | 1390/1455 (96%) | 938 (68%)  | 290 (21%) | 162 (12%) | 0           | 4  |
| 2   | B     | 1068/1224 (87%) | 727 (68%)  | 220 (21%) | 121 (11%) | 0           | 5  |
| 3   | C     | 264/268 (98%)   | 159 (60%)  | 66 (25%)  | 39 (15%)  | 0           | 3  |
| 4   | D     | 173/218 (79%)   | 122 (70%)  | 34 (20%)  | 17 (10%)  | 0           | 7  |
| 5   | E     | 212/215 (99%)   | 148 (70%)  | 49 (23%)  | 15 (7%)   | 1           | 11 |
| 6   | F     | 82/84 (98%)     | 64 (78%)   | 14 (17%)  | 4 (5%)    | 1           | 16 |
| 7   | G     | 169/171 (99%)   | 131 (78%)  | 26 (15%)  | 12 (7%)   | 1           | 11 |
| 8   | H     | 129/146 (88%)   | 84 (65%)   | 30 (23%)  | 15 (12%)  | 0           | 5  |
| 9   | I     | 114/122 (93%)   | 77 (68%)   | 30 (26%)  | 7 (6%)    | 1           | 13 |
| 10  | J     | 63/70 (90%)     | 37 (59%)   | 10 (16%)  | 16 (25%)  | 0           | 1  |
| 11  | K     | 112/120 (93%)   | 89 (80%)   | 18 (16%)  | 5 (4%)    | 2           | 17 |
| 12  | L     | 44/70 (63%)     | 19 (43%)   | 14 (32%)  | 11 (25%)  | 0           | 1  |
| All | All   | 3820/4163 (92%) | 2595 (68%) | 801 (21%) | 424 (11%) | 1           | 5  |

All (424) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | GLN  |
| 1   | A     | 48  | ALA  |
| 1   | A     | 54  | ASN  |
| 1   | A     | 55  | ASP  |
| 1   | A     | 57  | ARG  |
| 1   | A     | 62  | ASP  |
| 1   | A     | 65  | LEU  |
| 1   | A     | 74  | MET  |
| 1   | A     | 76  | GLU  |
| 1   | A     | 78  | PRO  |
| 1   | A     | 93  | VAL  |
| 1   | A     | 130 | ASP  |
| 1   | A     | 154 | SER  |
| 1   | A     | 167 | CYS  |
| 1   | A     | 250 | ILE  |
| 1   | A     | 255 | SER  |
| 1   | A     | 286 | HIS  |
| 1   | A     | 311 | GLN  |
| 1   | A     | 322 | VAL  |
| 1   | A     | 335 | ARG  |
| 1   | A     | 385 | ILE  |
| 1   | A     | 418 | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 423  | ASP  |
| 1   | A     | 424  | ILE  |
| 1   | A     | 536  | LEU  |
| 1   | A     | 567  | LYS  |
| 1   | A     | 619  | LYS  |
| 1   | A     | 626  | ASN  |
| 1   | A     | 666  | ILE  |
| 1   | A     | 775  | ILE  |
| 1   | A     | 968  | GLN  |
| 1   | A     | 1002 | GLY  |
| 1   | A     | 1036 | ARG  |
| 1   | A     | 1105 | SER  |
| 1   | A     | 1112 | PRO  |
| 1   | A     | 1223 | ASP  |
| 1   | A     | 1281 | ARG  |
| 1   | A     | 1314 | SER  |
| 1   | A     | 1341 | ILE  |
| 1   | A     | 1365 | TYR  |
| 1   | A     | 1366 | ARG  |
| 1   | A     | 1378 | GLN  |
| 1   | A     | 1397 | LEU  |
| 1   | A     | 1403 | GLU  |
| 1   | A     | 1405 | THR  |
| 1   | A     | 1438 | THR  |
| 2   | B     | 108  | VAL  |
| 2   | B     | 115  | GLN  |
| 2   | B     | 186  | GLU  |
| 2   | B     | 206  | ASN  |
| 2   | B     | 258  | LEU  |
| 2   | B     | 259  | TYR  |
| 2   | B     | 334  | ILE  |
| 2   | B     | 367  | LEU  |
| 2   | B     | 629  | ASP  |
| 2   | B     | 643  | ASP  |
| 2   | B     | 709  | ASP  |
| 2   | B     | 727  | LYS  |
| 2   | B     | 731  | VAL  |
| 2   | B     | 746  | SER  |
| 2   | B     | 751  | VAL  |
| 2   | B     | 881  | ASN  |
| 2   | B     | 891  | ASP  |
| 2   | B     | 907  | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 958  | GLN  |
| 2   | B     | 1006 | ILE  |
| 2   | B     | 1046 | PRO  |
| 2   | B     | 1069 | PHE  |
| 2   | B     | 1100 | ASP  |
| 2   | B     | 1108 | ARG  |
| 2   | B     | 1156 | ASP  |
| 2   | B     | 1171 | VAL  |
| 2   | B     | 1175 | LEU  |
| 2   | B     | 1181 | GLU  |
| 2   | B     | 1182 | CYS  |
| 2   | B     | 1183 | LYS  |
| 2   | B     | 1186 | ASP  |
| 2   | B     | 1188 | LYS  |
| 3   | C     | 56   | THR  |
| 3   | C     | 78   | GLU  |
| 3   | C     | 91   | HIS  |
| 3   | C     | 141  | GLY  |
| 3   | C     | 149  | LYS  |
| 3   | C     | 156  | THR  |
| 3   | C     | 161  | LYS  |
| 3   | C     | 184  | ASN  |
| 3   | C     | 202  | PRO  |
| 3   | C     | 209  | TYR  |
| 3   | C     | 213  | PRO  |
| 3   | C     | 214  | ASN  |
| 3   | C     | 215  | GLU  |
| 3   | C     | 231  | ASN  |
| 3   | C     | 240  | VAL  |
| 4   | D     | 6    | SER  |
| 4   | D     | 8    | PHE  |
| 4   | D     | 12   | ARG  |
| 4   | D     | 19   | GLU  |
| 4   | D     | 20   | GLU  |
| 4   | D     | 21   | GLU  |
| 4   | D     | 52   | LEU  |
| 4   | D     | 131  | GLU  |
| 4   | D     | 177  | VAL  |
| 4   | D     | 192  | LYS  |
| 4   | D     | 199  | ASN  |
| 5   | E     | 106  | GLN  |
| 5   | E     | 130  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 62  | LEU  |
| 7   | G     | 63  | PRO  |
| 7   | G     | 139 | ILE  |
| 8   | H     | 81  | PRO  |
| 8   | H     | 128 | ASN  |
| 8   | H     | 140 | ALA  |
| 9   | I     | 3   | THR  |
| 9   | I     | 9   | ASP  |
| 9   | I     | 106 | CYS  |
| 10  | J     | 2   | ILE  |
| 10  | J     | 6   | ARG  |
| 10  | J     | 8   | PHE  |
| 10  | J     | 9   | SER  |
| 10  | J     | 17  | LYS  |
| 10  | J     | 28  | ASP  |
| 10  | J     | 32  | GLU  |
| 10  | J     | 64  | ASN  |
| 12  | L     | 50  | ASP  |
| 12  | L     | 53  | HIS  |
| 12  | L     | 59  | ALA  |
| 1   | A     | 4   | GLN  |
| 1   | A     | 42  | ASP  |
| 1   | A     | 44  | THR  |
| 1   | A     | 59  | GLY  |
| 1   | A     | 61  | ILE  |
| 1   | A     | 66  | LYS  |
| 1   | A     | 70  | CYS  |
| 1   | A     | 101 | LYS  |
| 1   | A     | 111 | GLY  |
| 1   | A     | 113 | LEU  |
| 1   | A     | 244 | PRO  |
| 1   | A     | 263 | THR  |
| 1   | A     | 290 | GLU  |
| 1   | A     | 312 | PRO  |
| 1   | A     | 318 | SER  |
| 1   | A     | 333 | GLU  |
| 1   | A     | 336 | ILE  |
| 1   | A     | 364 | VAL  |
| 1   | A     | 409 | SER  |
| 1   | A     | 421 | ALA  |
| 1   | A     | 483 | ASP  |
| 1   | A     | 661 | GLY  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 753  | GLY  |
| 1   | A     | 765  | VAL  |
| 1   | A     | 780  | VAL  |
| 1   | A     | 789  | LYS  |
| 1   | A     | 818  | MET  |
| 1   | A     | 824  | LEU  |
| 1   | A     | 846  | GLU  |
| 1   | A     | 847  | ASP  |
| 1   | A     | 875  | ALA  |
| 1   | A     | 986  | ILE  |
| 1   | A     | 1008 | GLN  |
| 1   | A     | 1016 | THR  |
| 1   | A     | 1106 | LEU  |
| 1   | A     | 1110 | LEU  |
| 1   | A     | 1123 | LEU  |
| 1   | A     | 1165 | GLU  |
| 1   | A     | 1212 | VAL  |
| 1   | A     | 1221 | LYS  |
| 1   | A     | 1233 | ASP  |
| 1   | A     | 1335 | ILE  |
| 1   | A     | 1377 | THR  |
| 1   | A     | 1386 | ARG  |
| 1   | A     | 1389 | PHE  |
| 2   | B     | 21   | GLU  |
| 2   | B     | 28   | GLU  |
| 2   | B     | 45   | SER  |
| 2   | B     | 46   | GLN  |
| 2   | B     | 114  | PRO  |
| 2   | B     | 229  | ALA  |
| 2   | B     | 260  | GLY  |
| 2   | B     | 266  | ALA  |
| 2   | B     | 282  | ILE  |
| 2   | B     | 308  | TRP  |
| 2   | B     | 513  | GLN  |
| 2   | B     | 559  | SER  |
| 2   | B     | 641  | GLU  |
| 2   | B     | 655  | LYS  |
| 2   | B     | 869  | SER  |
| 2   | B     | 888  | GLY  |
| 2   | B     | 1003 | ALA  |
| 2   | B     | 1035 | ALA  |
| 2   | B     | 1041 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1126 | GLY  |
| 2   | B     | 1153 | GLU  |
| 2   | B     | 1155 | SER  |
| 2   | B     | 1157 | ALA  |
| 2   | B     | 1167 | GLY  |
| 2   | B     | 1176 | ASN  |
| 2   | B     | 1178 | ASN  |
| 3   | C     | 84   | ARG  |
| 3   | C     | 87   | PHE  |
| 3   | C     | 110  | THR  |
| 3   | C     | 142  | VAL  |
| 3   | C     | 164  | ALA  |
| 3   | C     | 169  | LYS  |
| 3   | C     | 175  | ALA  |
| 3   | C     | 216  | GLY  |
| 3   | C     | 255  | VAL  |
| 3   | C     | 264  | GLN  |
| 4   | D     | 15   | LEU  |
| 4   | D     | 218  | GLU  |
| 5   | E     | 36   | GLU  |
| 5   | E     | 44   | ALA  |
| 5   | E     | 59   | SER  |
| 5   | E     | 73   | PRO  |
| 5   | E     | 74   | ASP  |
| 5   | E     | 192  | ARG  |
| 5   | E     | 206  | GLY  |
| 6   | F     | 81   | THR  |
| 7   | G     | 118  | ASP  |
| 7   | G     | 154  | VAL  |
| 8   | H     | 32   | THR  |
| 8   | H     | 59   | ILE  |
| 8   | H     | 82   | PRO  |
| 8   | H     | 84   | ALA  |
| 8   | H     | 92   | ASP  |
| 8   | H     | 107  | VAL  |
| 9   | I     | 57   | GLY  |
| 9   | I     | 62   | ILE  |
| 10  | J     | 14   | VAL  |
| 10  | J     | 29   | GLU  |
| 10  | J     | 33   | GLY  |
| 11  | K     | 53   | ASP  |
| 12  | L     | 35   | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 58   | LEU  |
| 1   | A     | 71   | GLN  |
| 1   | A     | 117  | GLU  |
| 1   | A     | 131  | SER  |
| 1   | A     | 170  | THR  |
| 1   | A     | 219  | PHE  |
| 1   | A     | 223  | GLY  |
| 1   | A     | 232  | GLU  |
| 1   | A     | 253  | ASN  |
| 1   | A     | 278  | THR  |
| 1   | A     | 317  | LYS  |
| 1   | A     | 357  | PRO  |
| 1   | A     | 399  | HIS  |
| 1   | A     | 419  | LYS  |
| 1   | A     | 439  | ASN  |
| 1   | A     | 465  | TYR  |
| 1   | A     | 517  | ASN  |
| 1   | A     | 543  | LEU  |
| 1   | A     | 592  | ASP  |
| 1   | A     | 605  | MET  |
| 1   | A     | 731  | ARG  |
| 1   | A     | 817  | ALA  |
| 1   | A     | 940  | ARG  |
| 1   | A     | 1164 | PRO  |
| 1   | A     | 1309 | ASP  |
| 1   | A     | 1411 | GLU  |
| 2   | B     | 58   | THR  |
| 2   | B     | 383  | ASN  |
| 2   | B     | 450  | ALA  |
| 2   | B     | 459  | TYR  |
| 2   | B     | 512  | ARG  |
| 2   | B     | 571  | PRO  |
| 2   | B     | 590  | HIS  |
| 2   | B     | 591  | ARG  |
| 2   | B     | 605  | ARG  |
| 2   | B     | 648  | HIS  |
| 2   | B     | 682  | SER  |
| 2   | B     | 711  | GLU  |
| 2   | B     | 738  | PHE  |
| 2   | B     | 792  | MET  |
| 2   | B     | 797  | TYR  |
| 2   | B     | 848  | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 878  | GLN  |
| 2   | B     | 884  | ARG  |
| 2   | B     | 943  | SER  |
| 2   | B     | 1017 | ILE  |
| 2   | B     | 1082 | MET  |
| 3   | C     | 60   | ASP  |
| 3   | C     | 89   | GLU  |
| 3   | C     | 93   | ASP  |
| 3   | C     | 167  | HIS  |
| 5   | E     | 115  | ASN  |
| 7   | G     | 53   | ASN  |
| 8   | H     | 17   | PRO  |
| 8   | H     | 77   | ARG  |
| 8   | H     | 108  | SER  |
| 8   | H     | 135  | LEU  |
| 9   | I     | 78   | CYS  |
| 10  | J     | 24   | LEU  |
| 10  | J     | 51   | LEU  |
| 10  | J     | 55   | ASP  |
| 11  | K     | 54   | ARG  |
| 11  | K     | 88   | LYS  |
| 12  | L     | 40   | LEU  |
| 12  | L     | 54   | ARG  |
| 1   | A     | 69   | THR  |
| 1   | A     | 276  | LEU  |
| 1   | A     | 283  | GLY  |
| 1   | A     | 400  | PRO  |
| 1   | A     | 756  | ILE  |
| 1   | A     | 795  | GLU  |
| 1   | A     | 910  | PRO  |
| 1   | A     | 958  | VAL  |
| 1   | A     | 1011 | GLN  |
| 1   | A     | 1028 | THR  |
| 1   | A     | 1104 | PRO  |
| 1   | A     | 1240 | CYS  |
| 1   | A     | 1242 | VAL  |
| 1   | A     | 1297 | GLU  |
| 2   | B     | 67   | SER  |
| 2   | B     | 68   | THR  |
| 2   | B     | 100  | PRO  |
| 2   | B     | 124  | TYR  |
| 2   | B     | 257  | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 369  | GLY  |
| 2   | B     | 419  | THR  |
| 2   | B     | 594  | ALA  |
| 2   | B     | 620  | ARG  |
| 2   | B     | 735  | ALA  |
| 2   | B     | 883  | LEU  |
| 2   | B     | 951  | GLN  |
| 2   | B     | 1011 | ILE  |
| 2   | B     | 1097 | HIS  |
| 2   | B     | 1144 | ALA  |
| 3   | C     | 77   | ILE  |
| 3   | C     | 198  | ALA  |
| 4   | D     | 30   | GLY  |
| 7   | G     | 19   | GLY  |
| 7   | G     | 26   | LEU  |
| 8   | H     | 44   | VAL  |
| 8   | H     | 52   | GLN  |
| 9   | I     | 47   | GLU  |
| 10  | J     | 27   | GLU  |
| 11  | K     | 29   | ASN  |
| 12  | L     | 43   | THR  |
| 12  | L     | 56   | LEU  |
| 12  | L     | 60   | ARG  |
| 1   | A     | 68   | GLN  |
| 1   | A     | 84   | ILE  |
| 1   | A     | 128  | ILE  |
| 1   | A     | 226  | GLU  |
| 1   | A     | 598  | LEU  |
| 1   | A     | 599  | SER  |
| 1   | A     | 633  | VAL  |
| 1   | A     | 648  | ASN  |
| 1   | A     | 649  | ILE  |
| 1   | A     | 739  | ASP  |
| 1   | A     | 755  | PHE  |
| 1   | A     | 841  | LEU  |
| 1   | A     | 871  | ASP  |
| 1   | A     | 969  | GLN  |
| 1   | A     | 1054 | LEU  |
| 1   | A     | 1266 | THR  |
| 2   | B     | 27   | ALA  |
| 2   | B     | 48   | LEU  |
| 2   | B     | 65   | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 197  | PHE  |
| 2   | B     | 309  | GLN  |
| 2   | B     | 414  | ALA  |
| 2   | B     | 418  | LYS  |
| 2   | B     | 530  | GLY  |
| 2   | B     | 636  | PRO  |
| 2   | B     | 758  | PHE  |
| 2   | B     | 766  | ARG  |
| 2   | B     | 867  | GLY  |
| 2   | B     | 1016 | ALA  |
| 3   | C     | 108  | GLU  |
| 4   | D     | 168  | LYS  |
| 5   | E     | 40   | GLU  |
| 5   | E     | 45   | LYS  |
| 6   | F     | 112  | GLU  |
| 6   | F     | 150  | GLU  |
| 7   | G     | 34   | VAL  |
| 7   | G     | 115  | MET  |
| 1   | A     | 245  | PRO  |
| 1   | A     | 492  | PRO  |
| 1   | A     | 525  | GLN  |
| 1   | A     | 1057 | VAL  |
| 1   | A     | 1158 | PRO  |
| 1   | A     | 1396 | ALA  |
| 2   | B     | 313  | MET  |
| 2   | B     | 364  | ILE  |
| 2   | B     | 480  | SER  |
| 2   | B     | 611  | PRO  |
| 2   | B     | 836  | GLU  |
| 2   | B     | 1214 | PRO  |
| 3   | C     | 18   | VAL  |
| 3   | C     | 176  | ILE  |
| 3   | C     | 230  | MET  |
| 4   | D     | 69   | ALA  |
| 4   | D     | 139  | LYS  |
| 5   | E     | 158  | SER  |
| 10  | J     | 63   | TYR  |
| 11  | K     | 90   | ALA  |
| 12  | L     | 28   | LYS  |
| 12  | L     | 46   | VAL  |
| 1   | A     | 196  | GLU  |
| 1   | A     | 300  | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 627  | GLY  |
| 2   | B     | 712  | PRO  |
| 3   | C     | 172  | PRO  |
| 3   | C     | 212  | PRO  |
| 1   | A     | 652  | VAL  |
| 1   | A     | 653  | VAL  |
| 2   | B     | 501  | PRO  |
| 5   | E     | 37   | LEU  |
| 1   | A     | 546  | VAL  |
| 1   | A     | 825  | ILE  |
| 1   | A     | 1379 | GLY  |
| 1   | A     | 1454 | MET  |
| 2   | B     | 411  | PRO  |
| 2   | B     | 551  | PRO  |
| 2   | B     | 1018 | PRO  |
| 3   | C     | 171  | GLY  |
| 2   | B     | 524  | PRO  |
| 2   | B     | 818  | PRO  |
| 3   | C     | 126  | GLY  |
| 6   | F     | 131  | PRO  |
| 7   | G     | 20   | PRO  |
| 7   | G     | 116  | PRO  |
| 2   | B     | 592  | ASN  |
| 5   | E     | 129  | PRO  |

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | A     | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 1274:ARG  | C      | 1275:GLY  | N      | 10.90        |
| 1     | A     | 1131:THR  | C      | 1142:THR  | N      | 8.08         |

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5407. 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: 35



Y Index: 35



Z Index: 35

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: 41



Y Index: 35

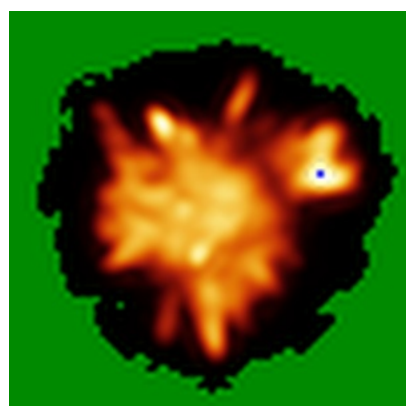


Z Index: 40

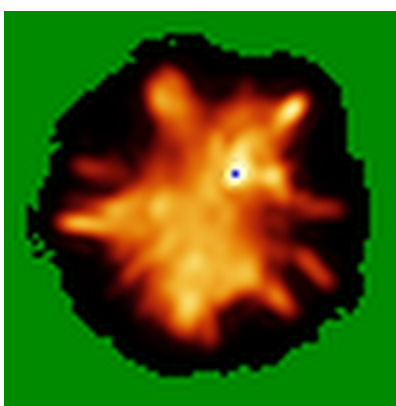
The images above show the largest variance slices of the map in three orthogonal directions.

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

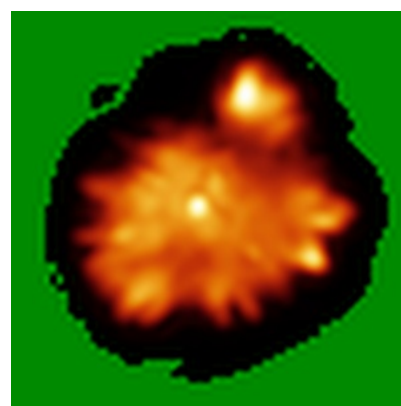
### 6.4.1 Primary map



X



Y

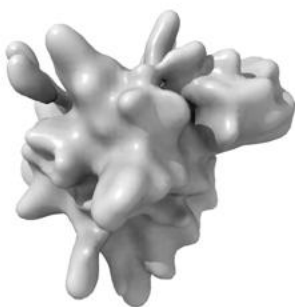


Z

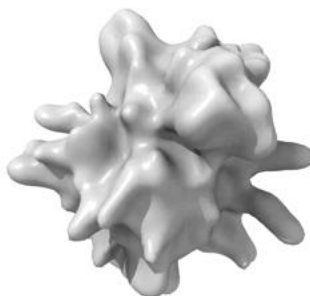
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

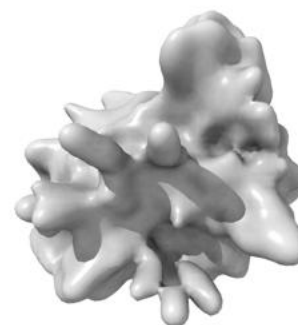
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

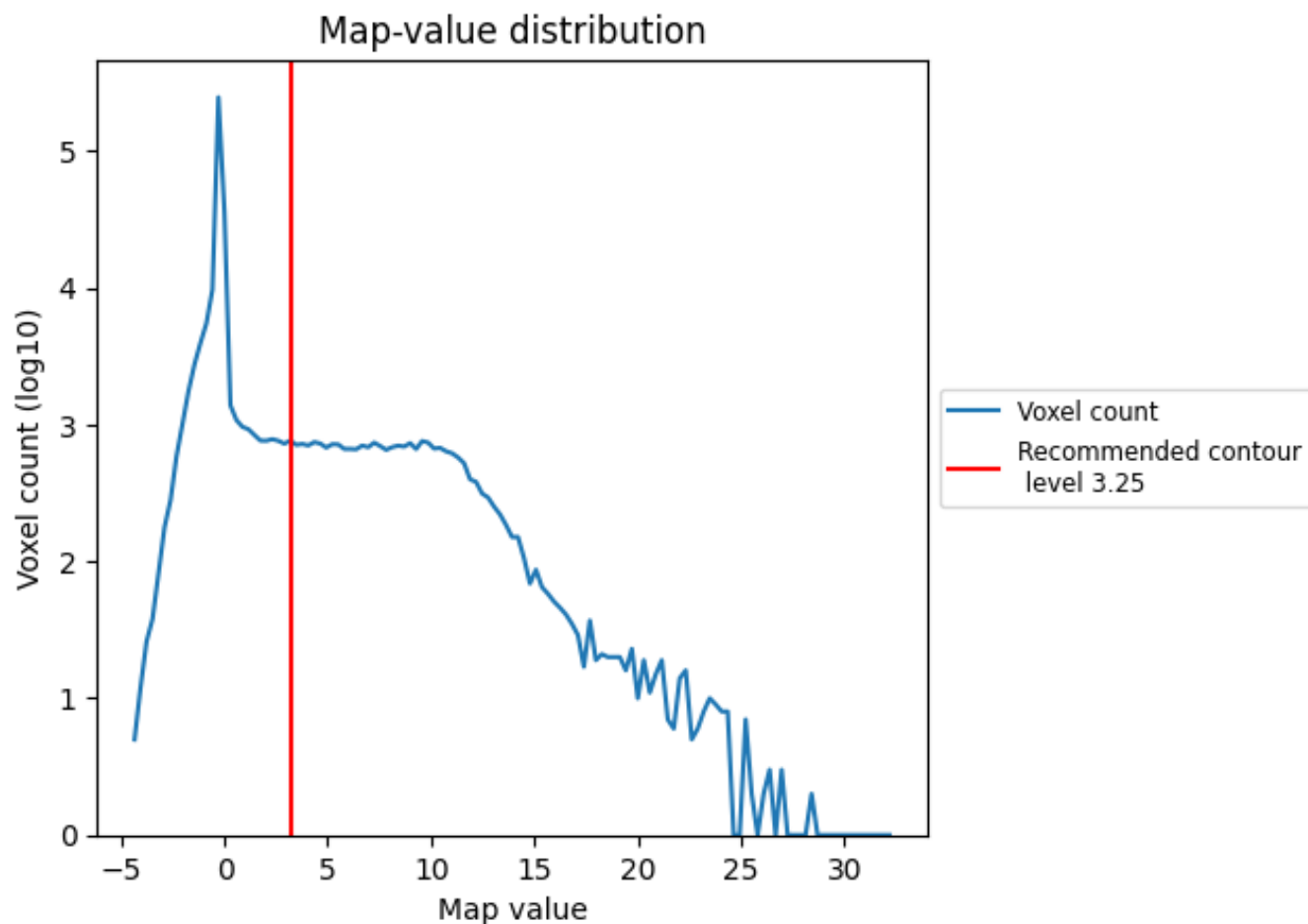
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

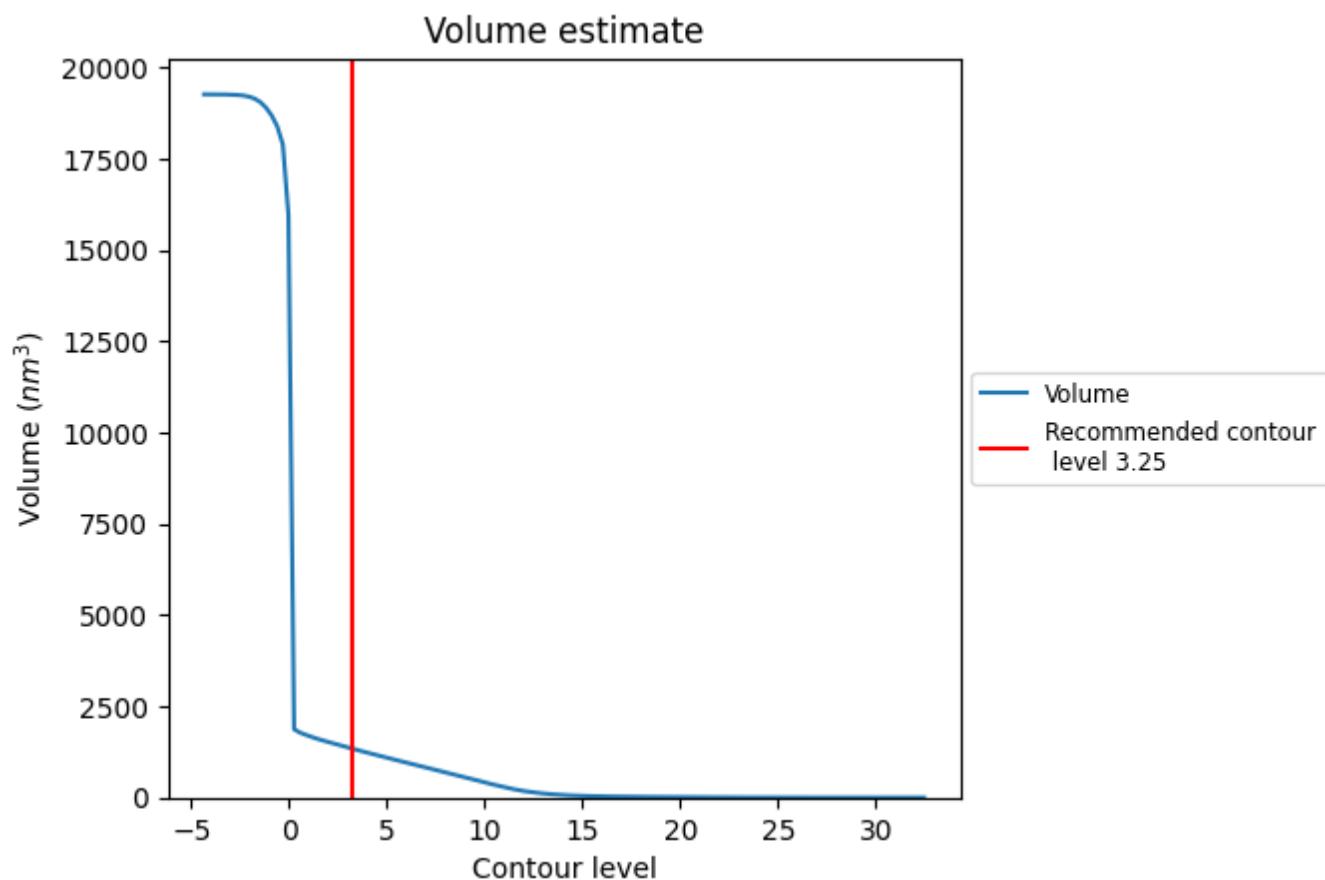
This section contains the results of statistical analysis of the map.

### 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.

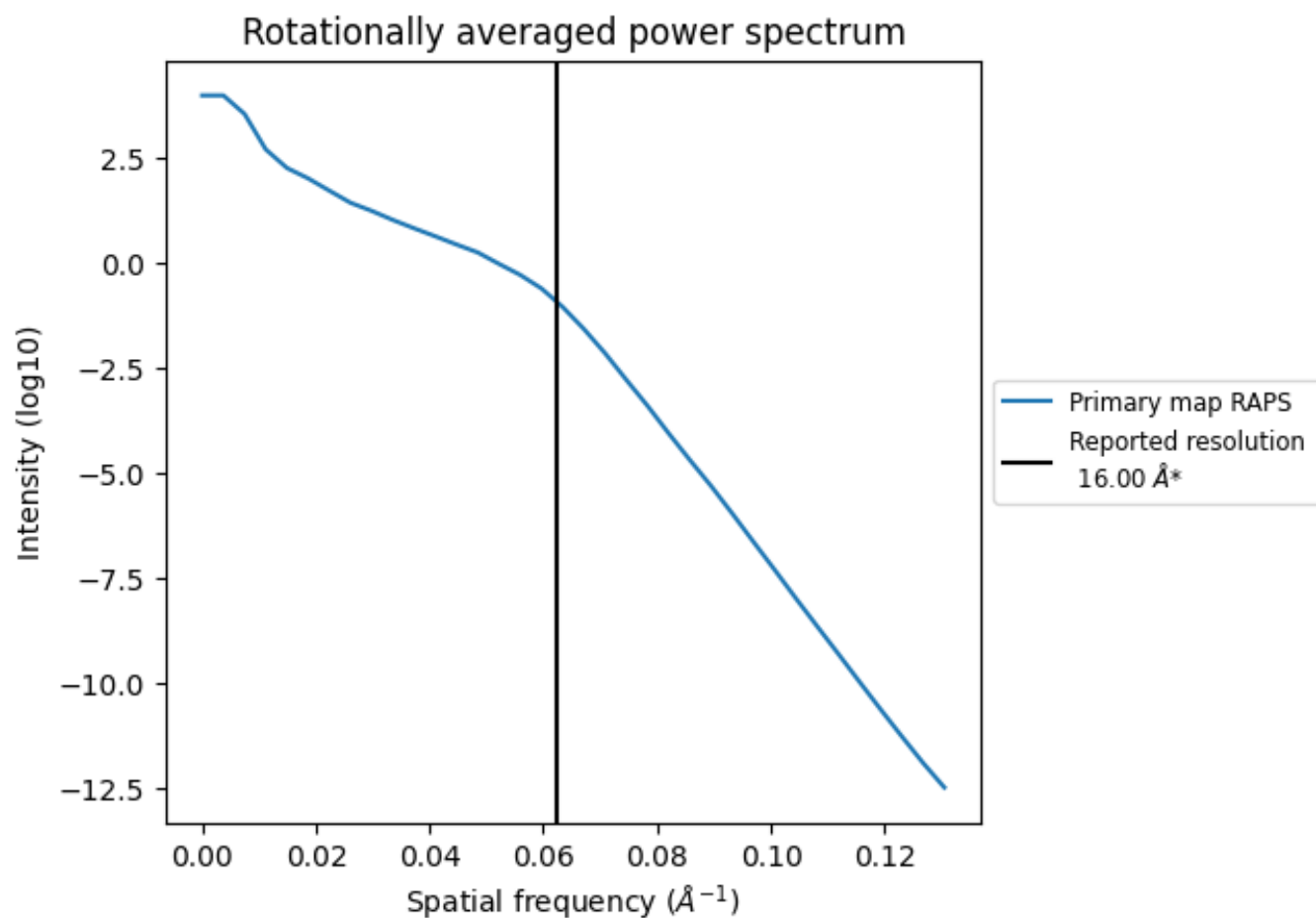
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1339 nm<sup>3</sup>; this corresponds to an approximate mass of 1210 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 0.062 Å<sup>-1</sup>

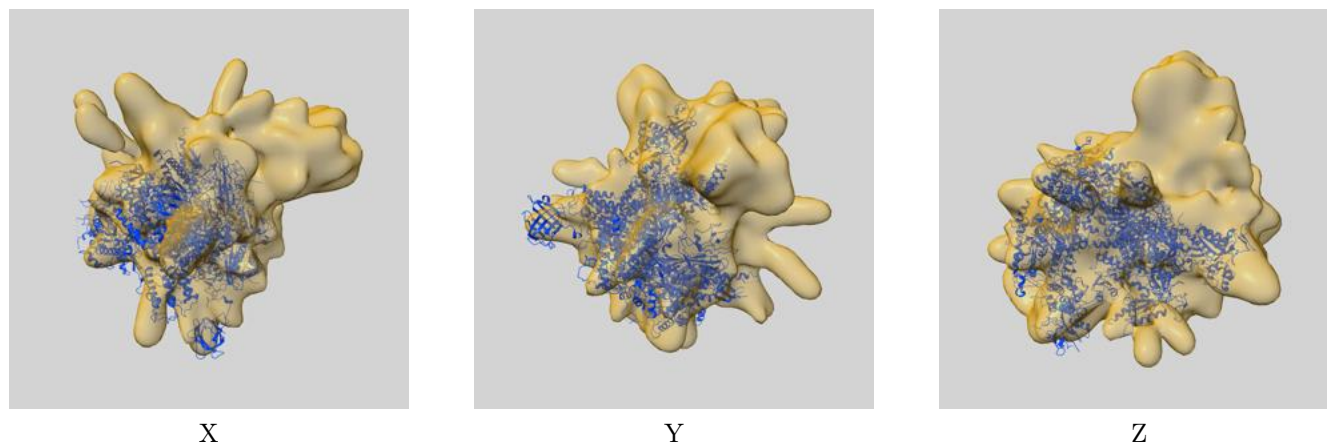
## 8 Fourier-Shell correlation ⓘ

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

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

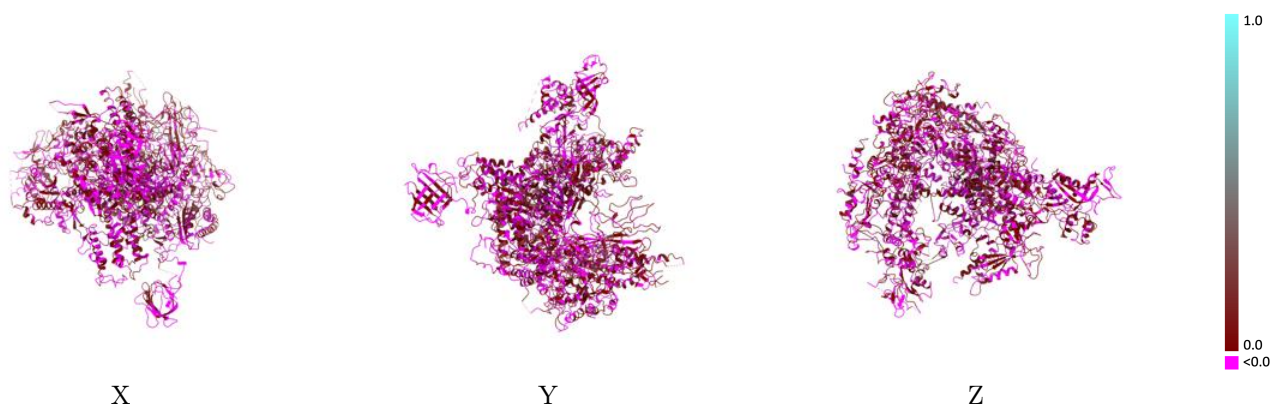
This section contains information regarding the fit between EMDB map EMD-5407 and PDB model 3J1N. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



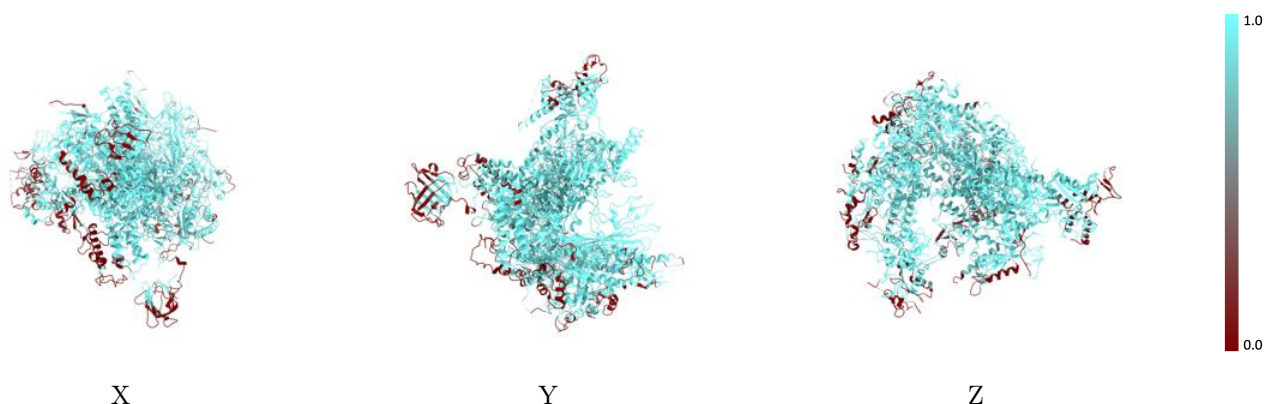
The images above show the 3D surface view of the map at the recommended contour level 3.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



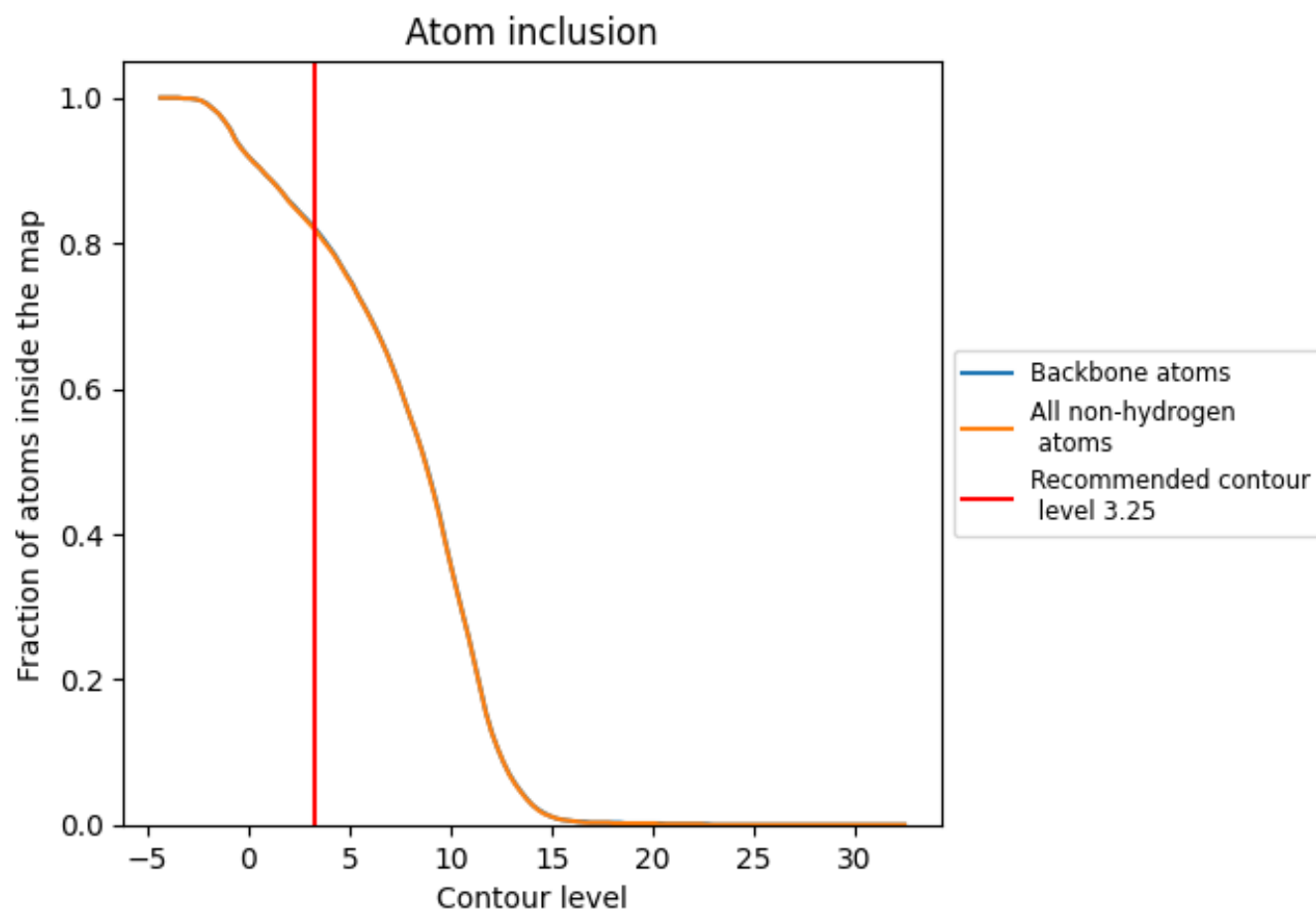
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.25).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% 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 (3.25) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                           | Q-score                                                                                   |
|-------|------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------|
| All   |  0.8200 |  0.0150  |
| A     |  0.8530 |  0.0170  |
| B     |  0.8990 |  0.0240  |
| C     |  0.6700 |  0.0100  |
| D     |  0.7480 |  0.0150  |
| E     |  0.7410 |  0.0070  |
| F     |  1.0000 |  0.0350  |
| G     |  0.7780 |  -0.0200 |
| H     |  0.3760 |  -0.0470 |
| I     |  0.8620 |  0.0560  |
| J     |  0.4580 |  -0.0390 |
| K     |  0.9500 |  0.0370  |
| L     |  0.6510 |  -0.0100 |

