



## Full wwPDB EM Validation Report ⓘ

Jun 11, 2024 – 02:44 PM JST

PDB ID : 7VBA  
EMDB ID : EMD-31876  
Title : Structure of the pre state human RNA Polymerase I Elongation Complex  
Authors : Zhao, D.; Liu, W.; Chen, K.; Yang, H.; Xu, Y.  
Deposited on : 2021-08-31  
Resolution : 2.89 Å(reported)

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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.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

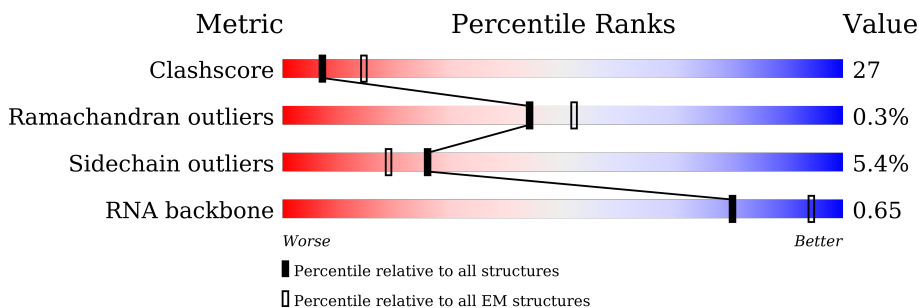
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.89 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) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 158937                      | 4297                        |
| Ramachandran outliers | 154571                      | 4023                        |
| Sidechain outliers    | 154315                      | 3826                        |
| RNA backbone          | 4643                        | 859                         |

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     | 1719   |                  |
| 2   | B     | 1135   |                  |
| 3   | C     | 346    |                  |
| 4   | E     | 210    |                  |
| 5   | F     | 127    |                  |
| 6   | H     | 150    |                  |
| 7   | I     | 126    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 8   | J     | 67     |                  |
| 9   | K     | 133    |                  |
| 10  | L     | 58     |                  |
| 11  | N     | 510    |                  |
| 12  | G     | 338    |                  |
| 13  | M     | 419    |                  |
| 14  | R     | 8      |                  |
| 15  | T     | 22     |                  |
| 16  | U     | 13     |                  |

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 33093 atoms, of which 14 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 I subunit RPA1.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 1473     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 11749 | 7474 | 2063 | 2134 | 78 |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 2   | B     | 1123     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 8912  | 5710 | 1517 | 1614 | 71 |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 337      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2697  | 1701 | 480 | 505 | 11 |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | E     | 199      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1641  | 1042 | 286 | 305 | 8 |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | F     | 76       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 610   | 392 | 103 | 110 | 5 |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | H     | 146      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1176  | 744 | 192 | 235 | 5 |         |       |

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA12.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | I     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 447   | 277 | 76 | 89 | 5 |         |       |

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | J     | 64       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 507   | 328 | 86 | 87 | 6 |         |       |

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | K     | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 863   | 535 | 156 | 165 | 7 |         |       |

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10  | L     | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 379   | 236 | 73 | 64 | 6 |         |       |

- Molecule 11 is a protein called DNA-directed RNA polymerase I subunit RPA34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | N     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1105  | 698 | 198 | 204 | 5 |         |       |

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA43.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | G     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1229  | 775 | 215 | 232 | 7 |         |       |

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | M     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 867   | 539 | 159 | 163 | 6 |         |       |

- Molecule 14 is a RNA chain called RNA (5'-R(P\*UP\*GP\*CP\*UP\*GP\*AP\*CP\*U)-3').

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 14  | R     | 8        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 168   | 75 | 27 | 58 | 8 |         |       |

- Molecule 15 is a DNA chain called DNA (5'-D(P\*GP\*CP\*CP\*AP\*GP\*AP\*GP\*AP\*CP\*AP\*GP\*CP\*GP\*AP\*GP\*TP\*CP\*AP\*GP\*CP\*AP\*A)-3').

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 15  | T     | 22       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 456   | 214 | 95 | 125 | 22 |         |       |

- Molecule 16 is a DNA chain called DNA (5'-D(P\*A\*CP\*TP\*GP\*TP\*CP\*CP\*TP\*CP\*TP\*GP\*GP\*C)-3').

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 16  | U     | 12       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 238   | 115 | 38 | 74 | 11 |         |       |

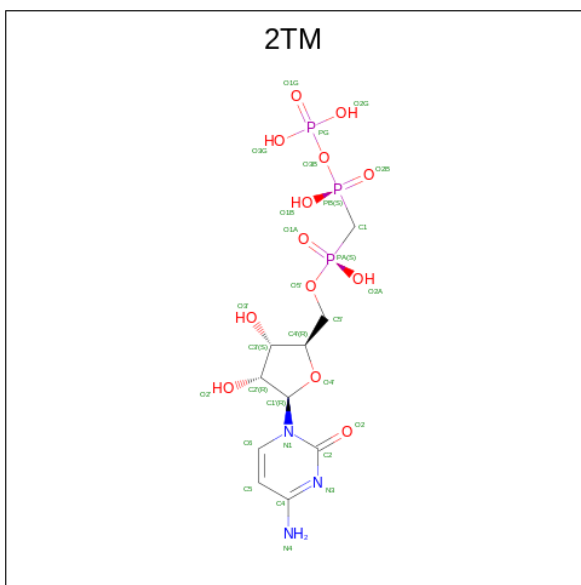
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 17  | A     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 17  | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 17  | J     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 17  | L     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 19 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (three-letter code: 2TM) (formula: C<sub>10</sub>H<sub>18</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>).

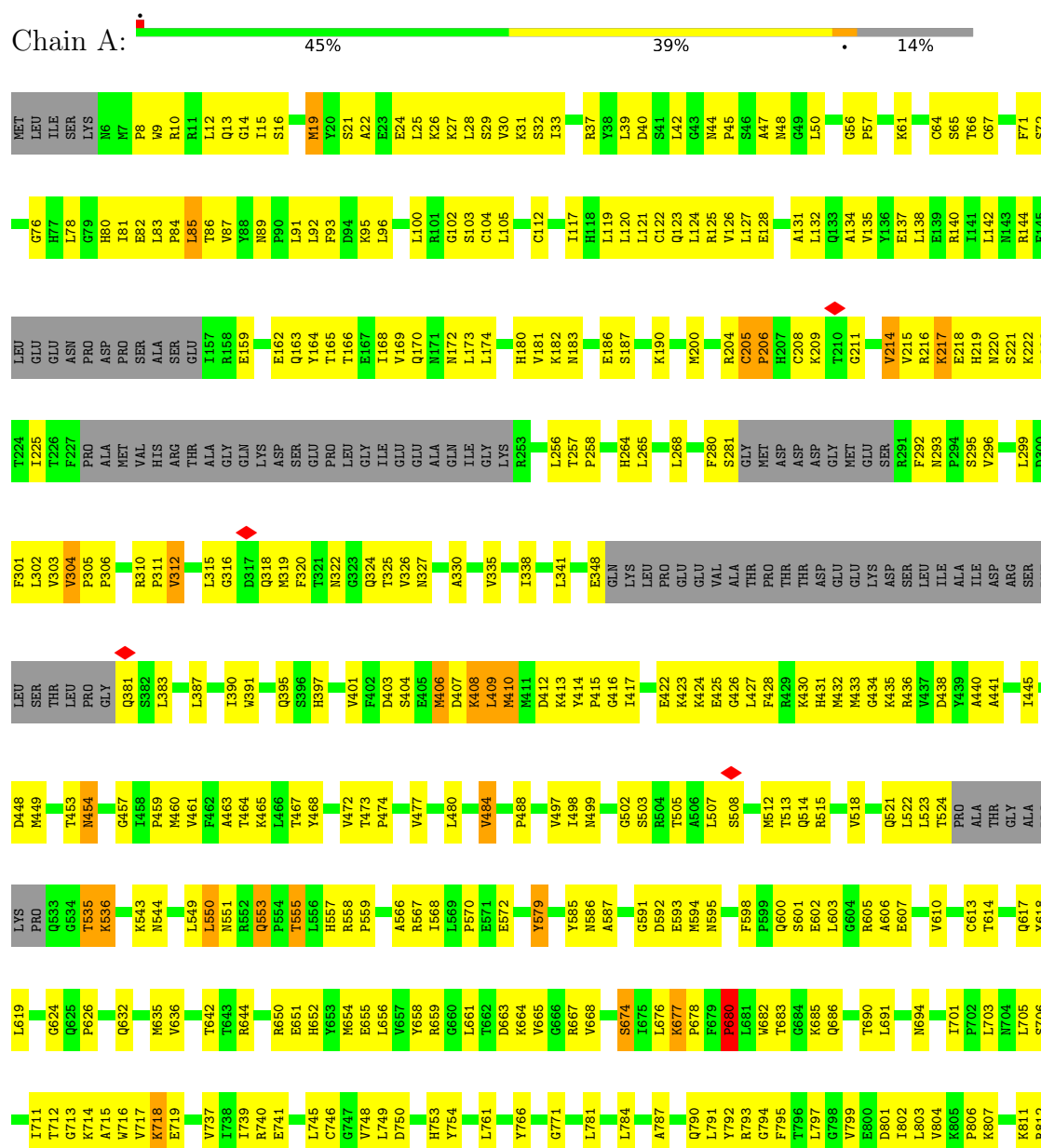


| Mol | Chain | Residues | Atoms |    |    |   |    | AltConf |   |
|-----|-------|----------|-------|----|----|---|----|---------|---|
| 19  | A     | 1        | Total | C  | H  | N | O  | P       | 0 |
|     |       |          | 43    | 10 | 14 | 3 | 13 | 3       |   |

### 3 Residue-property plots

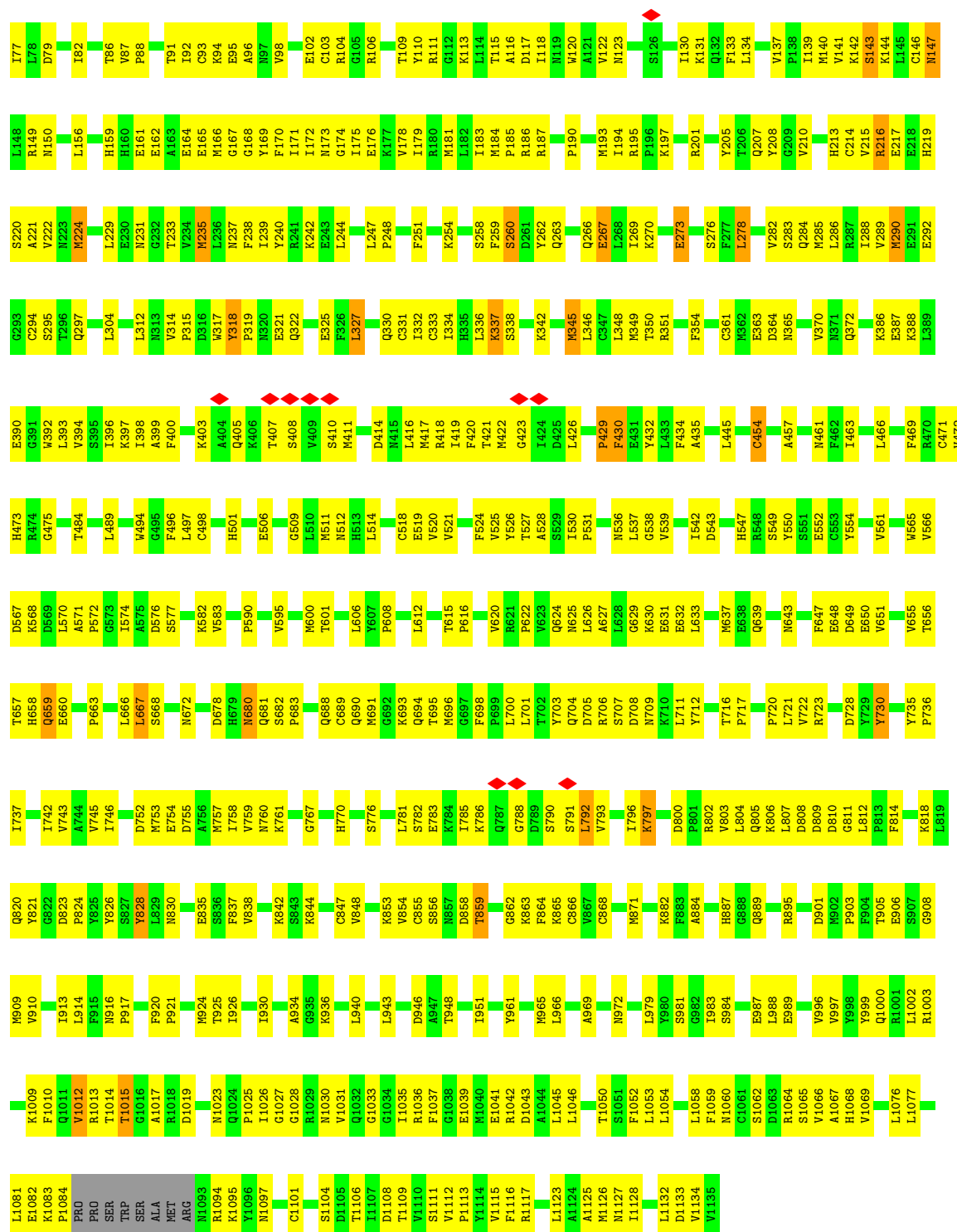
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 I subunit RPA1

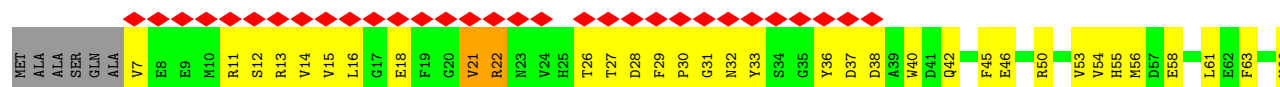


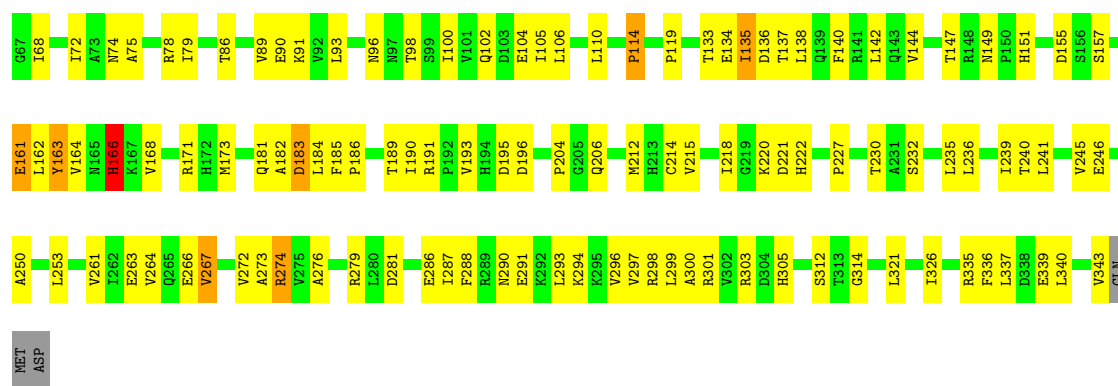






• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1





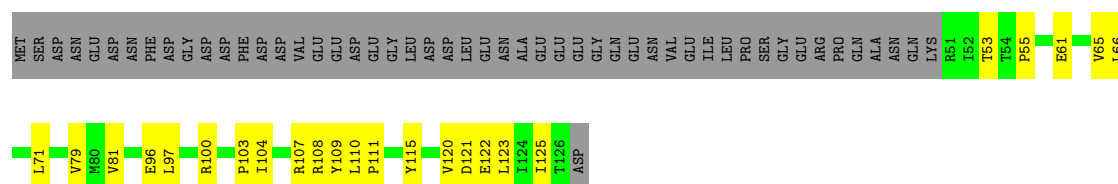
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 46% 48% 5%



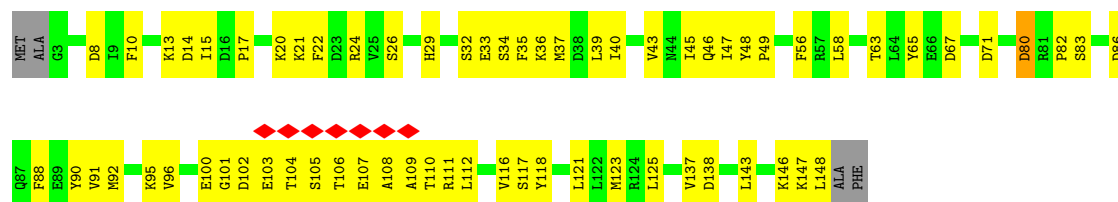
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 41% 19% 40%



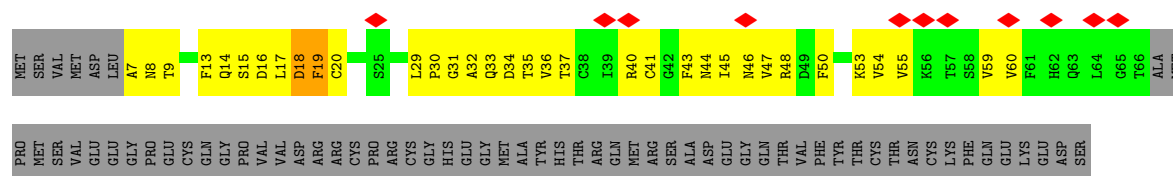
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 5% 53% 44%

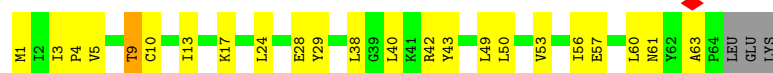


- Molecule 7: DNA-directed RNA polymerase I subunit RPA12

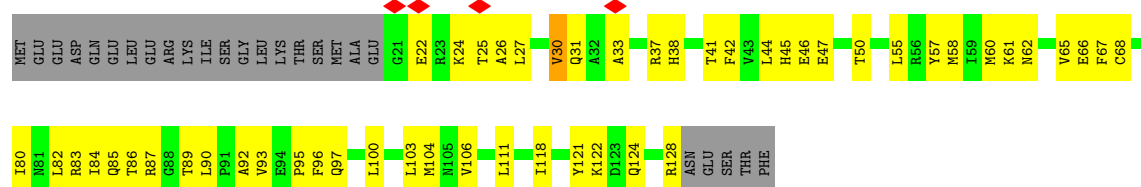
Chain I: 9% 21% 25% 52%



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



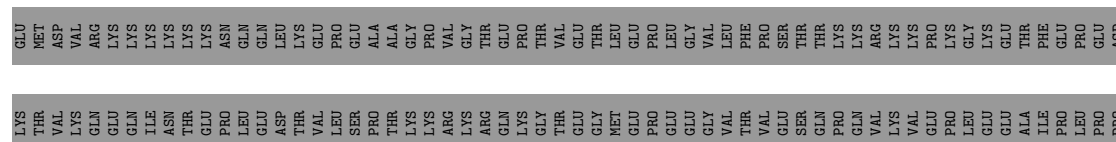
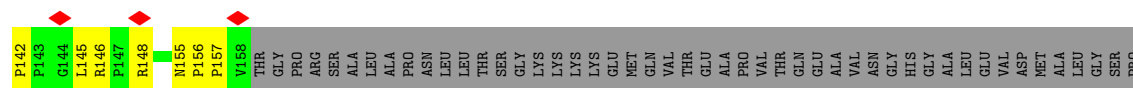
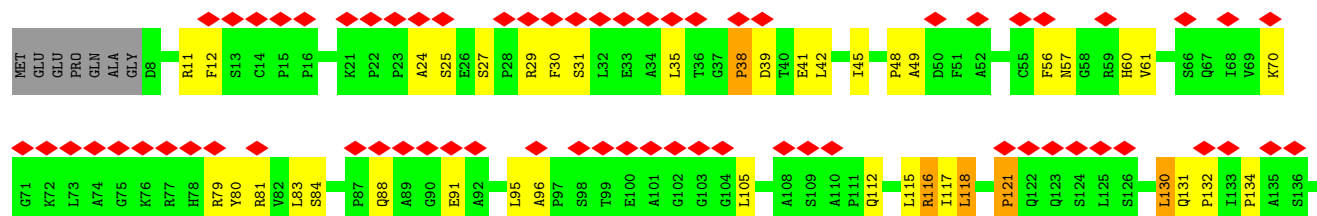
- Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC2



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

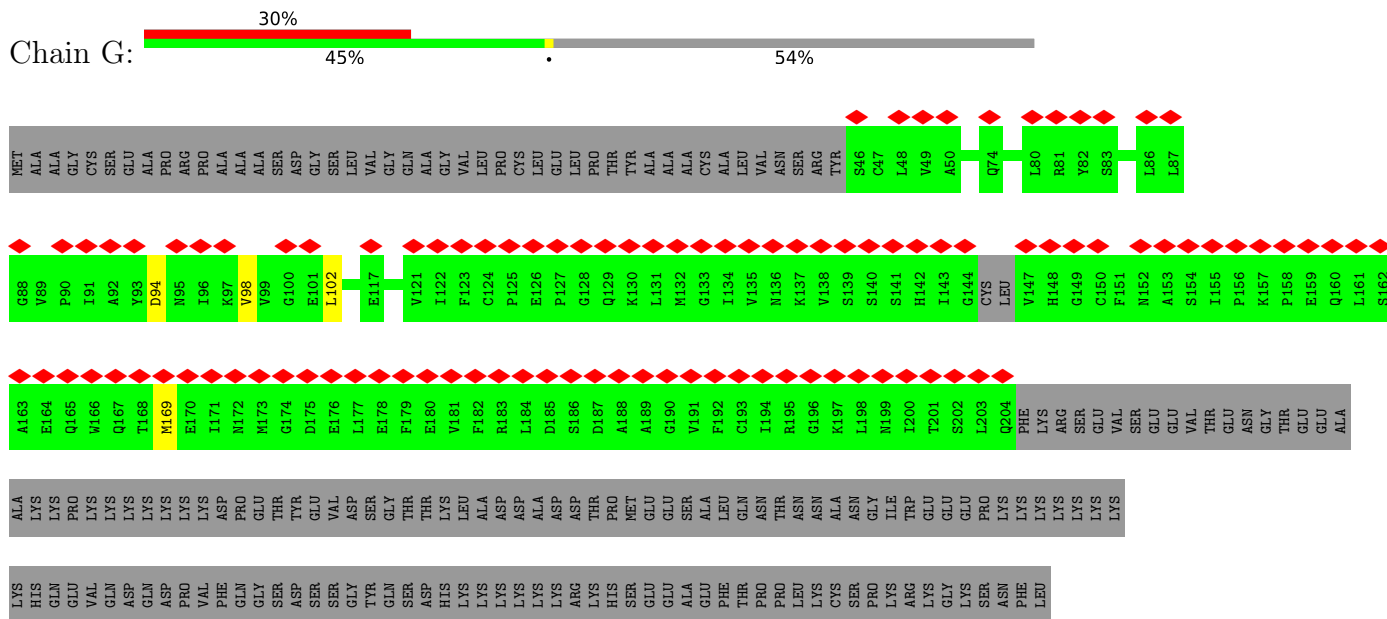


- Molecule 11: DNA-directed RNA polymerase I subunit RPA34

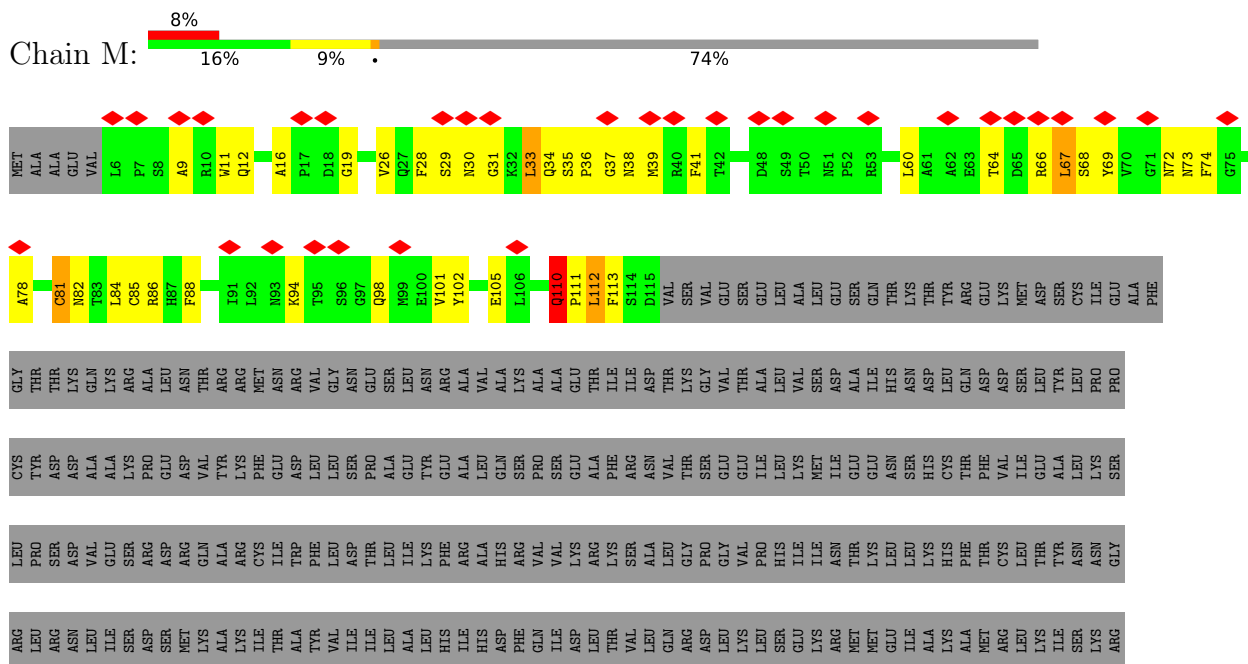


|     |     |     |     |
|-----|-----|-----|-----|
| GLN | GLN | GLY | THR |
| GLN | GLY | LYS | LYS |
| PRO | GLN | GLU | ARG |
| VAL | GLY | LYS | LYS |
|     | ALA | GLN | LYS |
|     | ARG | ASP | GLU |
|     | ALA | THR | GLN |
|     | PRO | VAL | MET |
|     | GLY | GLU | ALA |
|     | SER | PRO | MET |
|     | THR | GLU | MET |
|     | LYS | THR | GLU |
|     | LYS | GLU | PRO |
|     | ARG | VAL | GLY |
|     | LYS | VAL | THR |
|     | GLN | GLY | GLU |
|     | GLN | PRO | ALA |
|     | SER | GLU | MET |
|     | GLN | LEU | GLU |
|     | GLU | PRO | PRO |
|     | SER | ASP | VAL |
|     | ARG | ASP | GLU |
|     | MET | LEU | PRO |
|     | PRO | GLU | GLU |
|     | GLU | PRO | MET |
|     | THR | GLN | LYS |
|     | VAL | ALA | PRO |
|     | PRO | ALA | LEU |
|     | GLN | PRO | GLU |
|     | GLU | THR | GLU |
|     | GLU | SER | PRO |
|     | MET | THR | GLY |
|     | PRO | LYS | GLY |
|     | GLY | LYS | THR |
|     | PRO | LYS | MET |
|     | PRO | LYS | ALA |
|     | LEU | PRO | PRO |
|     | ASN | LYS | GLN |
|     | SER | LYS | GLN |
|     | GLU | GLU | PRO |
|     | SER | ARG | GLU |
|     | GLY | GLY | GLY |
|     | GLU | HIS | ALA |
|     | GLU | THR | LYS |
|     | ALA | VAL | PRO |
|     | PRO | THR | GLN |
|     | THR | GLU | ALA |
|     | GLY | PRO | GLN |
|     | ARG | ILE | ALA |
|     | ASP | GLN | ALA |
|     | LYS | PRO | LEU |
|     | LYS | LEU | ALA |
|     | ARG | GLU | ALA |
|     | LYS | PRO | PRO |
|     | GLN | GLU | LYS |
|     | GLN | LEU | LYS |
|     | GLN | PRO | LYS |

- Molecule 12: DNA-directed RNA polymerase I subunit RPA43



- Molecule 13: DNA-directed RNA polymerase I subunit RPA49



ARG VAL SER VAL ALA ALA GLY SER GLU GLU ASP HIS LYS LEU GLY THR LEU SER LEU LEU PRO PRO PRO ALA ALA GLN THR SER ASP ARG LEU ALA LYS ARG ARG LYS ILE THR

- Molecule 14: RNA (5'-R(P\*UP\*GP\*CP\*UP\*GP\*AP\*CP\*U)-3')

Chain R:  50% 38% 12%

U-8  
G-7  
C-6  
U-5  
U-1

- Molecule 15: DNA (5'-D(P\*GP\*CP\*CP\*AP\*GP\*AP\*GP\*AP\*CP\*AP\*GP\*CP\*GP\*AP\*GP\*TP\*CP\*AP\*GP\*CP\*AP\*A)-3')

Chain T:  45% 55%

G-11  
A-8  
G-7  
A-6  
G-5  
A-4  
C-3  
A-2  
G-1  
G3  
A6  
G7  
C8  
A9  
A10

- Molecule 16: DNA (5'-D(P\*A\*CP\*TP\*GP\*TP\*CP\*CP\*TP\*CP\*TP\*GP\*GP\*C)-3')

Chain U:  46% 46% 8%

DA  
C1  
T2  
G3  
T4  
C5  
C6  
T7  
C12

## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, Not provided       |           |
| Number of particles used             | 382890                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF         | Depositor |
| CTF correction method                | NONE                      | Depositor |
| Microscope                           | FEI TITAN KRIOS           | Depositor |
| Voltage (kV)                         | 300                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                        | Depositor |
| Minimum defocus (nm)                 | Not provided              |           |
| Maximum defocus (nm)                 | Not provided              |           |
| Magnification                        | Not provided              |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value                    | 5.648                     | Depositor |
| Minimum map value                    | -3.264                    | Depositor |
| Average map value                    | -0.002                    | Depositor |
| Map value standard deviation         | 0.151                     | Depositor |
| Recommended contour level            | 0.351                     | Depositor |
| Map size ( $\text{\AA}$ )            | 337.28, 337.28, 337.28    | wwPDB     |
| Map dimensions                       | 320, 320, 320             | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0          | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.054, 1.054, 1.054       | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.47         | 1/11988 (0.0%) | 0.69        | 4/16184 (0.0%)  |
| 2   | B     | 0.51         | 3/9127 (0.0%)  | 0.76        | 8/12350 (0.1%)  |
| 3   | C     | 0.50         | 0/2751         | 0.80        | 3/3729 (0.1%)   |
| 4   | E     | 0.32         | 0/1669         | 0.49        | 0/2254          |
| 5   | F     | 0.32         | 0/620          | 0.48        | 0/839           |
| 6   | H     | 0.38         | 0/1197         | 0.61        | 1/1614 (0.1%)   |
| 7   | I     | 0.38         | 0/454          | 0.65        | 0/615           |
| 8   | J     | 0.49         | 0/516          | 0.70        | 0/696           |
| 9   | K     | 0.34         | 0/878          | 0.61        | 0/1182          |
| 10  | L     | 0.33         | 0/385          | 0.55        | 0/511           |
| 11  | N     | 0.75         | 2/1140 (0.2%)  | 0.87        | 2/1560 (0.1%)   |
| 12  | G     | 0.33         | 0/1252         | 0.55        | 0/1691          |
| 13  | M     | 0.66         | 0/884          | 0.80        | 2/1192 (0.2%)   |
| 14  | R     | 0.37         | 0/186          | 0.90        | 0/287           |
| 15  | T     | 0.60         | 0/514          | 0.83        | 0/791           |
| 16  | U     | 0.55         | 0/264          | 1.04        | 0/405           |
| All | All   | 0.48         | 6/33825 (0.0%) | 0.71        | 20/45900 (0.0%) |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 11  | N     | 57  | ASN  | C-N   | 6.46  | 1.44        | 1.33     |
| 2   | B     | 283 | SER  | CA-CB | -5.78 | 1.44        | 1.52     |
| 11  | N     | 38  | PRO  | N-CD  | 5.76  | 1.55        | 1.47     |
| 2   | B     | 143 | SER  | CA-CB | -5.58 | 1.44        | 1.52     |
| 1   | A     | 674 | SER  | CA-CB | -5.44 | 1.44        | 1.52     |
| 2   | B     | 682 | SER  | CA-CB | -5.41 | 1.44        | 1.52     |

All (20) bond angle outliers are listed below:



| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | N     | 121  | PRO  | CA-N-CD | -8.62 | 99.43       | 111.50   |
| 2   | B     | 826  | TYR  | CB-CA-C | 5.98  | 122.36      | 110.40   |
| 2   | B     | 159  | HIS  | N-CA-C  | -5.81 | 95.31       | 111.00   |
| 1   | A     | 1598 | ARG  | N-CA-C  | -5.79 | 95.37       | 111.00   |
| 2   | B     | 1009 | LYS  | CB-CA-C | -5.76 | 98.88       | 110.40   |
| 1   | A     | 1182 | TYR  | CB-CA-C | 5.65  | 121.69      | 110.40   |
| 6   | H     | 22   | PHE  | CB-CA-C | 5.60  | 121.60      | 110.40   |
| 11  | N     | 155  | ASN  | C-N-CD  | -5.57 | 108.35      | 120.60   |
| 2   | B     | 730  | TYR  | CB-CA-C | -5.55 | 99.29       | 110.40   |
| 3   | C     | 166  | HIS  | CB-CA-C | 5.50  | 121.40      | 110.40   |
| 2   | B     | 266  | GLN  | CB-CA-C | 5.40  | 121.19      | 110.40   |
| 2   | B     | 147  | ASN  | CB-CA-C | 5.24  | 120.88      | 110.40   |
| 3   | C     | 191  | ARG  | CB-CA-C | -5.24 | 99.92       | 110.40   |
| 2   | B     | 216  | ARG  | CB-CA-C | -5.14 | 100.12      | 110.40   |
| 1   | A     | 579  | TYR  | CB-CA-C | -5.14 | 100.13      | 110.40   |
| 13  | M     | 82   | ASN  | CB-CA-C | 5.13  | 120.67      | 110.40   |
| 3   | C     | 163  | TYR  | CB-CA-C | -5.11 | 100.17      | 110.40   |
| 2   | B     | 351  | ARG  | CB-CA-C | 5.07  | 120.54      | 110.40   |
| 13  | M     | 110  | GLN  | CB-CA-C | -5.05 | 100.29      | 110.40   |
| 1   | A     | 680  | PRO  | N-CA-CB | -5.00 | 97.09       | 102.60   |

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     | 11749 | 0        | 11888    | 723     | 0            |
| 2   | B     | 8912  | 0        | 8896     | 553     | 0            |
| 3   | C     | 2697  | 0        | 2676     | 153     | 0            |
| 4   | E     | 1641  | 0        | 1671     | 110     | 0            |
| 5   | F     | 610   | 0        | 642      | 19      | 0            |
| 6   | H     | 1176  | 0        | 1137     | 57      | 0            |
| 7   | I     | 447   | 0        | 429      | 56      | 0            |
| 8   | J     | 507   | 0        | 523      | 25      | 0            |
| 9   | K     | 863   | 0        | 850      | 68      | 0            |
| 10  | L     | 379   | 0        | 387      | 24      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 11  | N     | 1105  | 0        | 1098     | 48      | 0            |
| 12  | G     | 1229  | 0        | 1212     | 0       | 0            |
| 13  | M     | 867   | 0        | 844      | 66      | 0            |
| 14  | R     | 168   | 0        | 85       | 3       | 0            |
| 15  | T     | 456   | 0        | 244      | 19      | 0            |
| 16  | U     | 238   | 0        | 138      | 6       | 0            |
| 17  | A     | 2     | 0        | 0        | 0       | 0            |
| 17  | B     | 1     | 0        | 0        | 0       | 0            |
| 17  | J     | 1     | 0        | 0        | 0       | 0            |
| 17  | L     | 1     | 0        | 0        | 0       | 0            |
| 18  | A     | 1     | 0        | 0        | 0       | 0            |
| 19  | A     | 29    | 14       | 14       | 0       | 0            |
| All | All   | 33079 | 14       | 32734    | 1695    | 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 27.

All (1695) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 11:N:142:PRO:CG  | 11:N:145:LEU:HD21 | 1.50                     | 1.42              |
| 11:N:142:PRO:HG2 | 11:N:145:LEU:CD2  | 1.54                     | 1.35              |
| 7:I:16:ASP:O     | 13:M:67:LEU:CD2   | 1.76                     | 1.33              |
| 1:A:408:LYS:NZ   | 1:A:409:LEU:HD22  | 1.46                     | 1.29              |
| 1:A:407:ASP:OD2  | 1:A:410:MET:HG3   | 1.40                     | 1.18              |
| 7:I:16:ASP:O     | 13:M:67:LEU:HD22  | 1.04                     | 1.18              |
| 1:A:408:LYS:HZ3  | 1:A:409:LEU:CD2   | 1.56                     | 1.17              |
| 1:A:408:LYS:NZ   | 1:A:409:LEU:CD2   | 2.06                     | 1.15              |
| 2:B:792:LEU:HB2  | 2:B:865:LYS:HD3   | 1.24                     | 1.15              |
| 13:M:67:LEU:HD21 | 13:M:69:TYR:CZ    | 1.83                     | 1.13              |
| 2:B:785:ILE:HG21 | 2:B:792:LEU:HD21  | 1.27                     | 1.12              |
| 1:A:316:GLY:HA2  | 15:T:10:DA:H2"    | 1.28                     | 1.09              |
| 1:A:521:GLN:HA   | 1:A:524:THR:HB    | 1.36                     | 1.07              |
| 2:B:14:PRO:HD3   | 2:B:946:ASP:HB3   | 1.36                     | 1.05              |
| 3:C:267:VAL:HG12 | 3:C:272:VAL:CG1   | 1.86                     | 1.05              |
| 1:A:312:VAL:HG21 | 1:A:320:PHE:HB3   | 1.34                     | 1.05              |
| 2:B:73:ILE:HB    | 2:B:75:PHE:CZ     | 1.91                     | 1.04              |
| 3:C:291:GLU:HA   | 3:C:294:LYS:HE3   | 1.36                     | 1.04              |
| 3:C:267:VAL:HG12 | 3:C:272:VAL:HG12  | 1.36                     | 1.02              |
| 1:A:754:TYR:CE1  | 1:A:781:LEU:HD13  | 1.95                     | 1.01              |
| 13:M:67:LEU:HD21 | 13:M:69:TYR:OH    | 1.59                     | 1.00              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:881:MET:HG3   | 1:A:910:MET:HG2   | 1.39                     | 1.00              |
| 1:A:408:LYS:HZ3   | 1:A:409:LEU:HD22  | 0.96                     | 0.98              |
| 1:A:132:LEU:HG    | 4:E:210:GLN:HE22  | 1.27                     | 0.98              |
| 7:I:16:ASP:OD1    | 13:M:67:LEU:HD23  | 1.62                     | 0.97              |
| 4:E:72:MET:HE2    | 4:E:103:LEU:HB2   | 1.47                     | 0.96              |
| 2:B:785:ILE:CG2   | 2:B:792:LEU:HD21  | 1.95                     | 0.96              |
| 1:A:969:MET:HG3   | 2:B:489:LEU:HD22  | 1.47                     | 0.95              |
| 1:A:1282:LYS:HE3  | 1:A:1564:LEU:HD13 | 1.49                     | 0.94              |
| 2:B:709:ASN:ND2   | 15:T:7:DG:H5"     | 1.80                     | 0.94              |
| 1:A:1512:ILE:HG21 | 1:A:1515:TYR:HE1  | 1.28                     | 0.93              |
| 2:B:10:LEU:HD12   | 2:B:11:PRO:HD2    | 1.48                     | 0.93              |
| 11:N:35:LEU:HD22  | 11:N:42:LEU:HD21  | 1.50                     | 0.93              |
| 13:M:12:GLN:OE1   | 13:M:98:GLN:NE2   | 2.01                     | 0.93              |
| 2:B:88:PRO:HD2    | 2:B:92:ILE:HD12   | 1.51                     | 0.92              |
| 1:A:1145:PRO:HD2  | 4:E:204:ILE:HD11  | 1.52                     | 0.92              |
| 2:B:396:ILE:HG22  | 2:B:422:MET:HB2   | 1.48                     | 0.92              |
| 1:A:1090:LEU:HD22 | 4:E:30:GLN:HG2    | 1.51                     | 0.91              |
| 1:A:939:GLU:HG2   | 1:A:940:PRO:HD2   | 1.48                     | 0.91              |
| 6:H:104:THR:HG22  | 6:H:107:GLU:HB3   | 1.54                     | 0.90              |
| 1:A:122:CYS:HB3   | 1:A:165:THR:HG21  | 1.53                     | 0.90              |
| 2:B:600:MET:HB3   | 2:B:608:PRO:HB3   | 1.54                     | 0.90              |
| 13:M:67:LEU:HD21  | 13:M:69:TYR:CE1   | 2.05                     | 0.90              |
| 3:C:54:VAL:HG21   | 3:C:279:ARG:NH2   | 1.87                     | 0.89              |
| 11:N:146:ARG:HH12 | 11:N:148:ARG:HH22 | 1.17                     | 0.89              |
| 1:A:316:GLY:CA    | 15:T:10:DA:H2"    | 2.03                     | 0.88              |
| 1:A:1313:GLN:HE22 | 1:A:1535:LYS:HB2  | 1.37                     | 0.88              |
| 1:A:754:TYR:HE1   | 1:A:781:LEU:HD13  | 1.32                     | 0.88              |
| 1:A:869:VAL:HG21  | 1:A:918:GLN:HE21  | 1.39                     | 0.88              |
| 1:A:1580:THR:HG22 | 1:A:1582:GLY:H    | 1.35                     | 0.88              |
| 2:B:73:ILE:HB     | 2:B:75:PHE:HZ     | 1.39                     | 0.88              |
| 5:F:79:VAL:HG12   | 5:F:81:VAL:HG12   | 1.53                     | 0.88              |
| 2:B:792:LEU:HB2   | 2:B:865:LYS:CD    | 2.04                     | 0.88              |
| 1:A:407:ASP:OD2   | 1:A:410:MET:CG    | 2.22                     | 0.87              |
| 2:B:408:SER:HA    | 2:B:411:MET:HB2   | 1.56                     | 0.87              |
| 2:B:403:LYS:HB2   | 2:B:418:ARG:HH12  | 1.40                     | 0.86              |
| 7:I:40:ARG:HD2    | 7:I:43:PHE:HA     | 1.55                     | 0.86              |
| 2:B:216:ARG:HB2   | 2:B:334:ILE:HG22  | 1.54                     | 0.86              |
| 2:B:392:TRP:HE1   | 2:B:423:GLY:HA2   | 1.39                     | 0.85              |
| 13:M:28:PHE:CE1   | 13:M:33:LEU:HD11  | 2.11                     | 0.85              |
| 2:B:68:PHE:HA     | 2:B:405:GLN:HE22  | 1.42                     | 0.84              |
| 4:E:94:MET:HG2    | 4:E:99:ILE:HD11   | 1.58                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:117:ASP:HB3   | 2:B:131:LYS:HE2   | 1.57                     | 0.84              |
| 2:B:178:VAL:HB    | 2:B:457:ALA:HB2   | 1.60                     | 0.84              |
| 2:B:648:GLU:HG3   | 11:N:130:LEU:HD22 | 1.59                     | 0.84              |
| 4:E:85:LYS:O      | 4:E:89:VAL:HG13   | 1.78                     | 0.84              |
| 1:A:713:GLY:O     | 6:H:20:LYS:HE3    | 1.78                     | 0.83              |
| 1:A:860:MET:HE2   | 1:A:864:LYS:HE3   | 1.60                     | 0.83              |
| 2:B:781:LEU:HD22  | 2:B:792:LEU:HB3   | 1.60                     | 0.83              |
| 1:A:555:THR:HG21  | 2:B:1041:GLU:HG3  | 1.61                     | 0.83              |
| 2:B:1068:HIS:HB3  | 2:B:1109:THR:HA   | 1.61                     | 0.83              |
| 1:A:1334:ARG:HG3  | 1:A:1335:PRO:HD2  | 1.59                     | 0.83              |
| 1:A:912:ILE:HD11  | 2:B:924:MET:HG2   | 1.61                     | 0.83              |
| 1:A:1619:ARG:HH22 | 4:E:196:PRO:HD2   | 1.44                     | 0.82              |
| 2:B:400:PHE:HA    | 2:B:418:ARG:CZ    | 2.10                     | 0.82              |
| 4:E:110:MET:HE1   | 4:E:118:LEU:HD11  | 1.60                     | 0.82              |
| 2:B:796:ILE:HD11  | 2:B:807:LEU:HB2   | 1.60                     | 0.82              |
| 2:B:792:LEU:HD12  | 2:B:865:LYS:HD2   | 1.61                     | 0.82              |
| 3:C:91:LYS:HE2    | 10:L:54:VAL:HG11  | 1.62                     | 0.82              |
| 1:A:312:VAL:CG2   | 1:A:320:PHE:HB3   | 2.10                     | 0.81              |
| 2:B:14:PRO:CD     | 2:B:946:ASP:HB3   | 2.10                     | 0.81              |
| 2:B:260:SER:HB3   | 7:I:18:ASP:HB2    | 1.61                     | 0.81              |
| 1:A:1097:GLN:O    | 1:A:1101:LYS:HG2  | 1.81                     | 0.81              |
| 2:B:631:GLU:HG3   | 2:B:631:GLU:O     | 1.80                     | 0.81              |
| 1:A:1153:ASP:OD1  | 1:A:1154:ILE:N    | 2.12                     | 0.81              |
| 2:B:708:ASP:O     | 2:B:776:SER:HB3   | 1.80                     | 0.81              |
| 3:C:104:GLU:HG2   | 3:C:105:ILE:HD12  | 1.61                     | 0.81              |
| 2:B:940:LEU:HD12  | 8:J:43:TYR:HB3    | 1.63                     | 0.81              |
| 2:B:758:ILE:HB    | 2:B:914:LEU:HB2   | 1.62                     | 0.80              |
| 9:K:22:GLU:HG3    | 9:K:25:THR:H      | 1.44                     | 0.80              |
| 2:B:73:ILE:CB     | 2:B:75:PHE:CZ     | 2.65                     | 0.80              |
| 8:J:40:LEU:HD11   | 8:J:49:LEU:HD12   | 1.64                     | 0.80              |
| 1:A:1354:ILE:O    | 1:A:1357:LYS:HG2  | 1.81                     | 0.80              |
| 1:A:1531:LEU:HB3  | 1:A:1535:LYS:HE2  | 1.64                     | 0.80              |
| 1:A:403:ASP:HB3   | 1:A:406:MET:HE2   | 1.63                     | 0.79              |
| 2:B:567:ASP:OD1   | 2:B:568:LYS:N     | 2.15                     | 0.79              |
| 1:A:658:TYR:HB2   | 9:K:67:PHE:HZ     | 1.47                     | 0.79              |
| 2:B:700:LEU:HD11  | 2:B:706:ARG:HG3   | 1.63                     | 0.79              |
| 2:B:536:ASN:HA    | 11:N:48:PRO:HG3   | 1.64                     | 0.79              |
| 2:B:783:GLU:OE1   | 2:B:783:GLU:N     | 2.15                     | 0.79              |
| 2:B:396:ILE:HA    | 2:B:422:MET:HG3   | 1.62                     | 0.79              |
| 1:A:1512:ILE:HG21 | 1:A:1515:TYR:CE1  | 2.15                     | 0.79              |
| 3:C:102:GLN:HB2   | 3:C:105:ILE:HD13  | 1.65                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1036:ARG:NH1  | 15:T:3:DG:OP1     | 2.16                     | 0.79              |
| 1:A:404:SER:HB2   | 1:A:415:PRO:HA    | 1.65                     | 0.78              |
| 3:C:163:TYR:HD1   | 3:C:166:HIS:HB3   | 1.49                     | 0.78              |
| 2:B:856:SER:HB3   | 10:L:42:ARG:HB3   | 1.64                     | 0.78              |
| 1:A:659:ARG:HH22  | 1:A:790:GLN:NE2   | 1.81                     | 0.78              |
| 3:C:33:TYR:HB3    | 3:C:36:TYR:HB3    | 1.63                     | 0.78              |
| 1:A:310:ARG:HE    | 1:A:325:THR:HG22  | 1.48                     | 0.78              |
| 3:C:267:VAL:CG1   | 3:C:272:VAL:CG1   | 2.62                     | 0.78              |
| 1:A:8:PRO:HG3     | 2:B:1066:VAL:HG13 | 1.65                     | 0.78              |
| 2:B:92:ILE:HD11   | 2:B:859:THR:HA    | 1.66                     | 0.78              |
| 1:A:914:CYS:H     | 1:A:954:ARG:HD3   | 1.48                     | 0.78              |
| 2:B:758:ILE:CD1   | 2:B:895:ARG:HB2   | 2.13                     | 0.77              |
| 4:E:86:THR:O      | 4:E:89:VAL:HG22   | 1.84                     | 0.77              |
| 4:E:168:ASN:O     | 4:E:169:GLN:HB3   | 1.84                     | 0.77              |
| 1:A:425:GLU:HG3   | 1:A:426:GLY:H     | 1.48                     | 0.77              |
| 1:A:1288:VAL:HG21 | 1:A:1333:LEU:HD22 | 1.67                     | 0.77              |
| 1:A:1350:LEU:O    | 1:A:1354:ILE:HG12 | 1.83                     | 0.77              |
| 1:A:1531:LEU:HB3  | 1:A:1535:LYS:CE   | 2.15                     | 0.77              |
| 9:K:90:LEU:HD23   | 9:K:90:LEU:H      | 1.50                     | 0.76              |
| 1:A:122:CYS:CB    | 1:A:165:THR:HG21  | 2.16                     | 0.76              |
| 1:A:408:LYS:HZ2   | 1:A:409:LEU:HD22  | 1.48                     | 0.76              |
| 1:A:465:LYS:HZ2   | 2:B:1014:THR:HG22 | 1.50                     | 0.76              |
| 2:B:75:PHE:CD2    | 2:B:397:LYS:HE3   | 2.21                     | 0.76              |
| 1:A:430:LYS:HE3   | 1:A:431:HIS:HE1   | 1.51                     | 0.76              |
| 3:C:147:THR:H     | 3:C:164:VAL:HG22  | 1.50                     | 0.76              |
| 2:B:68:PHE:HA     | 2:B:405:GLN:NE2   | 1.99                     | 0.76              |
| 2:B:916:ASN:OD1   | 2:B:917:PRO:HD2   | 1.86                     | 0.76              |
| 5:F:81:VAL:HB     | 5:F:96:GLU:HG2    | 1.66                     | 0.76              |
| 15:T:-6:DA:H2'    | 15:T:-5:DG:C8     | 2.20                     | 0.76              |
| 13:M:67:LEU:HD12  | 13:M:68:SER:O     | 1.86                     | 0.75              |
| 2:B:73:ILE:CB     | 2:B:75:PHE:HZ     | 1.99                     | 0.75              |
| 1:A:939:GLU:HG2   | 1:A:940:PRO:CD    | 2.17                     | 0.75              |
| 1:A:1515:TYR:O    | 1:A:1516:GLN:HG2  | 1.85                     | 0.75              |
| 3:C:186:PRO:HG2   | 3:C:189:THR:OG1   | 1.86                     | 0.75              |
| 1:A:667:ARG:NH1   | 9:K:66:GLU:OE2    | 2.20                     | 0.75              |
| 1:A:668:VAL:H     | 9:K:85:GLN:HE22   | 1.32                     | 0.75              |
| 4:E:110:MET:CE    | 4:E:118:LEU:HD11  | 2.16                     | 0.75              |
| 11:N:88:GLN:O     | 11:N:91:GLU:HG3   | 1.86                     | 0.75              |
| 1:A:793:ARG:HG3   | 1:A:794:GLY:N     | 2.02                     | 0.74              |
| 1:A:31:LYS:NZ     | 1:A:48:ASN:OD1    | 2.21                     | 0.74              |
| 1:A:125:ARG:O     | 1:A:128:GLU:HG2   | 1.88                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:88:PRO:HD2    | 2:B:92:ILE:CD1    | 2.17                     | 0.74              |
| 2:B:170:PHE:O     | 2:B:176:GLU:HA    | 1.87                     | 0.74              |
| 1:A:1225:GLN:O    | 1:A:1226:MET:HB2  | 1.87                     | 0.74              |
| 2:B:1003:ARG:HD2  | 2:B:1003:ARG:O    | 1.87                     | 0.74              |
| 1:A:312:VAL:HG23  | 1:A:320:PHE:HA    | 1.70                     | 0.74              |
| 2:B:743:VAL:HG21  | 2:B:999:TYR:HE2   | 1.53                     | 0.73              |
| 3:C:27:THR:HA     | 3:C:32:ASN:ND2    | 2.03                     | 0.73              |
| 1:A:749:LEU:HB3   | 1:A:754:TYR:HE2   | 1.53                     | 0.73              |
| 1:A:650:ARG:HG2   | 1:A:654:MET:HE2   | 1.71                     | 0.73              |
| 1:A:1545:VAL:HG21 | 7:I:53:LYS:HE3    | 1.69                     | 0.73              |
| 2:B:1060:ASN:OD1  | 2:B:1064:ARG:NH1  | 2.20                     | 0.73              |
| 1:A:134:ALA:O     | 1:A:138:LEU:HD23  | 1.89                     | 0.73              |
| 1:A:1289:CYS:HA   | 1:A:1552:VAL:HA   | 1.71                     | 0.73              |
| 1:A:1295:GLN:O    | 7:I:59:VAL:HG12   | 1.89                     | 0.73              |
| 1:A:1615:GLU:HG3  | 4:E:193:ILE:HD13  | 1.71                     | 0.73              |
| 2:B:141:VAL:O     | 2:B:146:CYS:SG    | 2.46                     | 0.73              |
| 3:C:54:VAL:HG21   | 3:C:279:ARG:HH22  | 1.51                     | 0.73              |
| 1:A:1334:ARG:CG   | 1:A:1335:PRO:HD2  | 2.19                     | 0.73              |
| 1:A:911:GLN:HA    | 1:A:915:LEU:O     | 1.89                     | 0.72              |
| 3:C:267:VAL:HG12  | 3:C:272:VAL:HG11  | 1.68                     | 0.72              |
| 9:K:30:VAL:HG23   | 9:K:41:THR:HB     | 1.70                     | 0.72              |
| 1:A:1349:LEU:HD21 | 1:A:1547:LEU:HD11 | 1.72                     | 0.72              |
| 2:B:73:ILE:HB     | 2:B:75:PHE:CE2    | 2.24                     | 0.72              |
| 2:B:396:ILE:HA    | 2:B:422:MET:CG    | 2.19                     | 0.72              |
| 2:B:536:ASN:HA    | 11:N:48:PRO:CG    | 2.20                     | 0.72              |
| 1:A:1593:GLU:OE1  | 1:A:1593:GLU:N    | 2.21                     | 0.72              |
| 2:B:64:PHE:HE2    | 2:B:397:LYS:HB2   | 1.54                     | 0.72              |
| 8:J:57:GLU:O      | 8:J:61:ASN:ND2    | 2.21                     | 0.72              |
| 1:A:1328:GLN:NE2  | 1:A:1333:LEU:O    | 2.22                     | 0.72              |
| 2:B:403:LYS:HB3   | 2:B:418:ARG:HH22  | 1.52                     | 0.72              |
| 1:A:1335:PRO:O    | 1:A:1338:ILE:HG22 | 1.90                     | 0.72              |
| 2:B:92:ILE:HG22   | 2:B:93:CYS:H      | 1.53                     | 0.72              |
| 3:C:53:VAL:O      | 11:N:157:PRO:HD3  | 1.90                     | 0.72              |
| 4:E:61:LEU:HD13   | 4:E:73:PHE:HD1    | 1.55                     | 0.72              |
| 1:A:104:CYS:SG    | 1:A:211:GLY:HA3   | 2.30                     | 0.71              |
| 2:B:193:MET:SD    | 2:B:195:ARG:NH2   | 2.63                     | 0.71              |
| 1:A:713:GLY:O     | 6:H:20:LYS:CE     | 2.37                     | 0.71              |
| 2:B:73:ILE:CG2    | 2:B:75:PHE:CZ     | 2.74                     | 0.71              |
| 4:E:13:ILE:O      | 4:E:17:ILE:HG13   | 1.91                     | 0.71              |
| 1:A:850:HIS:O     | 1:A:855:GLN:NE2   | 2.24                     | 0.71              |
| 3:C:287:ILE:HD11  | 3:C:299:LEU:HD22  | 1.71                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:H:104:THR:CG2   | 6:H:107:GLU:HB3   | 2.21                     | 0.71              |
| 1:A:749:LEU:HD23  | 1:A:754:TYR:OH    | 1.90                     | 0.70              |
| 1:A:1545:VAL:HG21 | 7:I:53:LYS:CE     | 2.21                     | 0.70              |
| 1:A:430:LYS:HE3   | 1:A:431:HIS:CE1   | 2.25                     | 0.70              |
| 2:B:140:MET:CE    | 2:B:168:GLY:HA2   | 2.21                     | 0.70              |
| 1:A:1619:ARG:NH2  | 4:E:196:PRO:HD2   | 2.06                     | 0.70              |
| 2:B:576:ASP:OD1   | 2:B:577:SER:N     | 2.25                     | 0.70              |
| 2:B:622:PRO:HB3   | 2:B:631:GLU:OE2   | 1.91                     | 0.70              |
| 1:A:1686:MET:HG3  | 1:A:1687:LEU:HD12 | 1.74                     | 0.70              |
| 2:B:46:PHE:O      | 2:B:50:VAL:HG22   | 1.92                     | 0.70              |
| 2:B:717:PRO:HB2   | 2:B:736:PRO:HB2   | 1.74                     | 0.70              |
| 1:A:512:MET:SD    | 1:A:515:ARG:NH2   | 2.65                     | 0.70              |
| 6:H:104:THR:HB    | 6:H:109:ALA:HB2   | 1.74                     | 0.70              |
| 1:A:138:LEU:HD11  | 1:A:165:THR:HG23  | 1.72                     | 0.70              |
| 1:A:797:LEU:HD12  | 1:A:897:MET:HE3   | 1.73                     | 0.70              |
| 4:E:190:VAL:HG22  | 4:E:208:LEU:HD12  | 1.73                     | 0.70              |
| 6:H:96:VAL:HG22   | 6:H:116:VAL:HG22  | 1.73                     | 0.70              |
| 1:A:686:GLN:O     | 1:A:690:THR:HG22  | 1.92                     | 0.70              |
| 4:E:54:ARG:HD2    | 4:E:57:ASP:HB3    | 1.72                     | 0.70              |
| 1:A:793:ARG:HG3   | 1:A:794:GLY:H     | 1.57                     | 0.70              |
| 2:B:58:VAL:HA     | 2:B:61:ILE:HG13   | 1.71                     | 0.70              |
| 3:C:184:LEU:HD23  | 3:C:185:PHE:CE2   | 2.27                     | 0.70              |
| 1:A:1145:PRO:HD2  | 4:E:204:ILE:CD1   | 2.21                     | 0.69              |
| 1:A:1097:GLN:HA   | 1:A:1100:VAL:HG22 | 1.75                     | 0.69              |
| 2:B:394:VAL:O     | 2:B:398:ILE:HG12  | 1.91                     | 0.69              |
| 4:E:159:LEU:HD23  | 4:E:160:LEU:HD23  | 1.74                     | 0.69              |
| 6:H:101:GLY:HA2   | 6:H:112:LEU:HD23  | 1.74                     | 0.69              |
| 1:A:312:VAL:HG23  | 1:A:320:PHE:CA    | 2.22                     | 0.69              |
| 2:B:781:LEU:HD23  | 2:B:781:LEU:O     | 1.92                     | 0.69              |
| 3:C:267:VAL:CG1   | 3:C:272:VAL:HG11  | 2.22                     | 0.69              |
| 4:E:92:GLN:O      | 4:E:95:GLN:HG2    | 1.92                     | 0.69              |
| 4:E:93:ARG:NH1    | 4:E:97:GLU:OE2    | 2.26                     | 0.69              |
| 7:I:16:ASP:OD2    | 13:M:66:ARG:HB2   | 1.93                     | 0.69              |
| 3:C:53:VAL:C      | 11:N:157:PRO:HD3  | 2.13                     | 0.69              |
| 1:A:87:VAL:HB     | 1:A:395:GLN:HE22  | 1.58                     | 0.69              |
| 1:A:258:PRO:HD2   | 1:A:391:TRP:CZ3   | 2.27                     | 0.69              |
| 7:I:8:ASN:ND2     | 13:M:34:GLN:HG2   | 2.07                     | 0.69              |
| 2:B:392:TRP:O     | 2:B:396:ILE:HG23  | 1.93                     | 0.69              |
| 1:A:745:LEU:HD22  | 6:H:117:SER:OG    | 1.93                     | 0.69              |
| 2:B:651:VAL:HG13  | 2:B:656:THR:HG21  | 1.75                     | 0.69              |
| 1:A:691:LEU:HD22  | 1:A:784:LEU:HD22  | 1.74                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1024:LEU:HA   | 1:A:1203:SER:O    | 1.92                     | 0.68              |
| 1:A:1702:VAL:HG23 | 1:A:1704:LYS:HG3  | 1.76                     | 0.68              |
| 1:A:910:MET:O     | 1:A:911:GLN:HB3   | 1.94                     | 0.68              |
| 1:A:1516:GLN:HG3  | 1:A:1526:GLN:HG3  | 1.76                     | 0.68              |
| 2:B:400:PHE:CD1   | 2:B:418:ARG:HG2   | 2.29                     | 0.68              |
| 7:I:16:ASP:OD2    | 13:M:66:ARG:HD2   | 1.94                     | 0.68              |
| 1:A:44:ASN:HB2    | 1:A:45:PRO:HD2    | 1.74                     | 0.68              |
| 1:A:1262:PRO:HA   | 1:A:1603:ASN:HD21 | 1.58                     | 0.68              |
| 2:B:392:TRP:NE1   | 2:B:423:GLY:HA2   | 2.09                     | 0.68              |
| 3:C:291:GLU:CA    | 3:C:294:LYS:HE3   | 2.21                     | 0.68              |
| 1:A:140:ARG:HH11  | 1:A:144:ARG:HH12  | 1.42                     | 0.68              |
| 1:A:754:TYR:HE1   | 1:A:781:LEU:CD1   | 2.05                     | 0.68              |
| 1:A:806:PRO:O     | 1:A:807:LYS:HB3   | 1.93                     | 0.68              |
| 11:N:70:LYS:HG2   | 11:N:79:ARG:HG2   | 1.74                     | 0.68              |
| 1:A:843:ARG:NH1   | 1:A:939:GLU:OE2   | 2.27                     | 0.68              |
| 7:I:18:ASP:HB3    | 13:M:111:PRO:HG2  | 1.75                     | 0.68              |
| 8:J:1:MET:CE      | 8:J:56:ILE:HD13   | 2.24                     | 0.67              |
| 1:A:860:MET:CE    | 1:A:864:LYS:HE3   | 2.24                     | 0.67              |
| 2:B:75:PHE:CE1    | 2:B:120:TRP:HB2   | 2.29                     | 0.67              |
| 1:A:338:ILE:HG12  | 1:A:390:ILE:HD12  | 1.77                     | 0.67              |
| 1:A:1014:VAL:CG2  | 4:E:165:LEU:HD21  | 2.23                     | 0.67              |
| 2:B:690:GLN:OE1   | 2:B:694:GLN:NE2   | 2.27                     | 0.67              |
| 3:C:16:LEU:HD12   | 3:C:21:VAL:HG23   | 1.77                     | 0.67              |
| 1:A:13:GLN:O      | 2:B:1133:ASP:HB2  | 1.94                     | 0.67              |
| 1:A:1512:ILE:HD13 | 1:A:1529:VAL:HG22 | 1.77                     | 0.67              |
| 1:A:1515:TYR:CD1  | 1:A:1527:VAL:HG23 | 2.30                     | 0.67              |
| 1:A:1566:GLU:HA   | 1:A:1576:LEU:HD13 | 1.75                     | 0.67              |
| 3:C:138:LEU:HD12  | 3:C:181:GLN:HE22  | 1.57                     | 0.67              |
| 3:C:235:LEU:HB2   | 3:C:301:ARG:HD3   | 1.76                     | 0.67              |
| 1:A:166:THR:HA    | 1:A:169:VAL:HG22  | 1.77                     | 0.67              |
| 7:I:17:LEU:HD11   | 7:I:37:THR:OG1    | 1.94                     | 0.67              |
| 8:J:3:ILE:HD12    | 8:J:4:PRO:HD2     | 1.75                     | 0.67              |
| 11:N:48:PRO:HD3   | 11:N:117:ILE:O    | 1.95                     | 0.67              |
| 1:A:434:GLY:HA3   | 2:B:1036:ARG:NH2  | 2.10                     | 0.66              |
| 1:A:465:LYS:NZ    | 2:B:1014:THR:HG22 | 2.10                     | 0.66              |
| 1:A:916:LEU:HB2   | 1:A:953:GLY:O     | 1.96                     | 0.66              |
| 1:A:979:ALA:O     | 1:A:982:THR:HG22  | 1.95                     | 0.66              |
| 7:I:16:ASP:O      | 13:M:67:LEU:HD23  | 1.87                     | 0.66              |
| 1:A:430:LYS:HG2   | 1:A:431:HIS:ND1   | 2.11                     | 0.66              |
| 3:C:245:VAL:CG2   | 3:C:273:ALA:HB3   | 2.26                     | 0.66              |
| 4:E:127:LEU:O     | 4:E:128:GLU:HG3   | 1.95                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1066:VAL:O    | 2:B:1066:VAL:HG12 | 1.96                     | 0.66              |
| 5:F:79:VAL:CG1    | 5:F:81:VAL:HG12   | 2.25                     | 0.66              |
| 1:A:690:THR:O     | 1:A:694:ASN:ND2   | 2.27                     | 0.66              |
| 2:B:187:ARG:HD2   | 2:B:615:THR:HB    | 1.77                     | 0.66              |
| 6:H:48:TYR:OH     | 6:H:147:LYS:HG3   | 1.96                     | 0.66              |
| 9:K:42:PHE:CE1    | 9:K:84:ILE:HD12   | 2.31                     | 0.66              |
| 1:A:603:LEU:O     | 1:A:603:LEU:HD23  | 1.96                     | 0.66              |
| 2:B:709:ASN:HD21  | 15:T:7:DG:H5"     | 1.61                     | 0.66              |
| 2:B:806:LYS:HG2   | 2:B:824:PRO:HD2   | 1.78                     | 0.66              |
| 4:E:77:PRO:HD2    | 4:E:105:VAL:O     | 1.96                     | 0.66              |
| 2:B:403:LYS:HE2   | 2:B:418:ARG:NH2   | 2.11                     | 0.65              |
| 3:C:53:VAL:HG21   | 9:K:118:ILE:HD13  | 1.76                     | 0.65              |
| 7:I:33:GLN:HG3    | 7:I:34:ASP:OD1    | 1.96                     | 0.65              |
| 2:B:566:VAL:HG21  | 2:B:574:ILE:HD12  | 1.78                     | 0.65              |
| 4:E:94:MET:SD     | 4:E:102:ALA:HB2   | 2.37                     | 0.65              |
| 1:A:1566:GLU:HA   | 1:A:1576:LEU:CD1  | 2.26                     | 0.65              |
| 2:B:233:THR:HG23  | 2:B:285:MET:HG2   | 1.78                     | 0.65              |
| 4:E:84:ILE:O      | 4:E:88:LYS:HG2    | 1.95                     | 0.65              |
| 1:A:642:THR:O     | 1:A:685:LYS:HE2   | 1.96                     | 0.65              |
| 1:A:1034:PRO:HD3  | 1:A:1166:LYS:HD3  | 1.78                     | 0.65              |
| 1:A:1104:LYS:HB2  | 1:A:1116:GLY:HA2  | 1.78                     | 0.65              |
| 1:A:812:ARG:HD2   | 1:A:914:CYS:HA    | 1.78                     | 0.65              |
| 2:B:194:ILE:HG23  | 2:B:207:GLN:OE1   | 1.97                     | 0.65              |
| 6:H:102:ASP:OD2   | 6:H:111:ARG:HB2   | 1.96                     | 0.65              |
| 2:B:1042:ARG:NH1  | 2:B:1043:ASP:OD1  | 2.30                     | 0.65              |
| 11:N:112:GLN:OE1  | 11:N:112:GLN:N    | 2.30                     | 0.65              |
| 1:A:12:LEU:HD21   | 2:B:1132:LEU:HD13 | 1.78                     | 0.65              |
| 1:A:1104:LYS:CB   | 1:A:1116:GLY:HA2  | 2.27                     | 0.65              |
| 3:C:11:ARG:O      | 3:C:303:ARG:HD3   | 1.97                     | 0.65              |
| 1:A:173:LEU:O     | 1:A:174:LEU:HB3   | 1.96                     | 0.65              |
| 1:A:1006:THR:HG21 | 1:A:1008:ARG:HE   | 1.62                     | 0.65              |
| 1:A:1096:ILE:O    | 1:A:1100:VAL:HG13 | 1.97                     | 0.65              |
| 1:A:807:LYS:HG3   | 1:A:807:LYS:O     | 1.97                     | 0.65              |
| 2:B:709:ASN:HD22  | 15:T:7:DG:H5"     | 1.61                     | 0.65              |
| 2:B:785:ILE:HG21  | 2:B:792:LEU:CD2   | 2.17                     | 0.65              |
| 2:B:936:LYS:HG2   | 2:B:966:LEU:HD21  | 1.79                     | 0.65              |
| 7:I:14:GLN:NE2    | 7:I:32:ALA:HB3    | 2.11                     | 0.65              |
| 2:B:346:LEU:O     | 2:B:350:THR:HG23  | 1.97                     | 0.65              |
| 3:C:274:ARG:HB3   | 3:C:274:ARG:HH11  | 1.61                     | 0.65              |
| 1:A:132:LEU:CG    | 4:E:210:GLN:HE22  | 2.08                     | 0.64              |
| 1:A:1349:LEU:CD2  | 1:A:1547:LEU:HD11 | 2.26                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:110:MET:SD    | 4:E:118:LEU:HD11  | 2.37                     | 0.64              |
| 11:N:142:PRO:HG2  | 11:N:145:LEU:CG   | 2.27                     | 0.64              |
| 2:B:224:MET:HE1   | 2:B:346:LEU:HD21  | 1.80                     | 0.64              |
| 2:B:757:MET:HE3   | 2:B:759:VAL:CG2   | 2.27                     | 0.64              |
| 2:B:1028:GLY:O    | 2:B:1033:GLY:HA3  | 1.97                     | 0.64              |
| 1:A:1334:ARG:CD   | 1:A:1335:PRO:HD2  | 2.27                     | 0.64              |
| 4:E:20:LEU:HD11   | 4:E:24:ARG:HE     | 1.61                     | 0.64              |
| 10:L:21:GLU:OE1   | 10:L:21:GLU:N     | 2.31                     | 0.64              |
| 2:B:842:LYS:O     | 2:B:844:LYS:HE2   | 1.97                     | 0.64              |
| 2:B:909:MET:HG2   | 8:J:42:ARG:HD3    | 1.80                     | 0.64              |
| 1:A:1133:ARG:HG2  | 1:A:1133:ARG:O    | 1.97                     | 0.64              |
| 4:E:90:TYR:OH     | 4:E:104:ILE:HD13  | 1.97                     | 0.64              |
| 2:B:73:ILE:CG2    | 2:B:75:PHE:HZ     | 2.09                     | 0.64              |
| 1:A:137:GLU:HG2   | 1:A:164:TYR:OH    | 1.97                     | 0.64              |
| 1:A:658:TYR:HB2   | 9:K:67:PHE:CZ     | 2.31                     | 0.64              |
| 1:A:1119:GLU:OE1  | 1:A:1122:ARG:NH1  | 2.22                     | 0.64              |
| 1:A:1318:ARG:HD2  | 1:A:1524:TRP:HE3  | 1.63                     | 0.64              |
| 3:C:7:VAL:N       | 6:H:49:PRO:HD2    | 2.13                     | 0.64              |
| 10:L:34:ILE:O     | 10:L:34:ILE:HG22  | 1.98                     | 0.64              |
| 1:A:1516:GLN:HG3  | 1:A:1526:GLN:H    | 1.62                     | 0.63              |
| 1:A:607:GLU:OE2   | 1:A:1710:THR:HG21 | 1.98                     | 0.63              |
| 1:A:1313:GLN:HG2  | 1:A:1537:ASN:HD21 | 1.63                     | 0.63              |
| 2:B:400:PHE:HD1   | 2:B:418:ARG:HG2   | 1.61                     | 0.63              |
| 2:B:1013:ARG:NH2  | 2:B:1017:ALA:O    | 2.30                     | 0.63              |
| 4:E:9:ARG:HD2     | 4:E:132:GLN:HE21  | 1.64                     | 0.63              |
| 13:M:33:LEU:HD13  | 13:M:36:PRO:HB3   | 1.80                     | 0.63              |
| 1:A:316:GLY:HA2   | 15:T:10:DA:C2'    | 2.17                     | 0.63              |
| 1:A:939:GLU:CG    | 1:A:940:PRO:HD2   | 2.26                     | 0.63              |
| 2:B:190:PRO:HB3   | 2:B:349:MET:HG2   | 1.79                     | 0.63              |
| 1:A:221:SER:OG    | 1:A:395:GLN:HG3   | 1.99                     | 0.63              |
| 1:A:430:LYS:HG2   | 1:A:431:HIS:CE1   | 2.34                     | 0.63              |
| 1:A:749:LEU:HD23  | 1:A:754:TYR:CZ    | 2.32                     | 0.63              |
| 1:A:1534:MET:C    | 1:A:1535:LYS:HD2  | 2.19                     | 0.63              |
| 2:B:75:PHE:CD1    | 2:B:120:TRP:HB2   | 2.34                     | 0.63              |
| 2:B:538:GLY:O     | 11:N:116:ARG:NH2  | 2.31                     | 0.63              |
| 2:B:566:VAL:CG2   | 2:B:574:ILE:HD12  | 2.28                     | 0.63              |
| 4:E:185:ILE:HD12  | 4:E:191:VAL:HG11  | 1.80                     | 0.63              |
| 1:A:414:TYR:HB3   | 1:A:415:PRO:HD2   | 1.81                     | 0.63              |
| 1:A:823:GLY:HA2   | 1:A:865:PHE:HE1   | 1.64                     | 0.63              |
| 1:A:1322:LEU:HD13 | 7:I:60:VAL:HB     | 1.81                     | 0.63              |
| 2:B:1067:ALA:HB1  | 2:B:1076:LEU:HD11 | 1.81                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:15:VAL:HA     | 3:C:300:ALA:HB2   | 1.81                     | 0.63              |
| 1:A:1022:ASP:HB3  | 4:E:200:ALA:HB2   | 1.81                     | 0.63              |
| 1:A:1293:VAL:O    | 1:A:1294:LEU:HG   | 1.99                     | 0.63              |
| 1:A:85:LEU:HD22   | 1:A:391:TRP:HE1   | 1.63                     | 0.63              |
| 1:A:460:MET:HG3   | 1:A:570:PRO:HA    | 1.81                     | 0.63              |
| 4:E:59:THR:HG23   | 4:E:74:VAL:O      | 1.99                     | 0.63              |
| 2:B:171:ILE:HG23  | 2:B:174:GLY:HA2   | 1.81                     | 0.62              |
| 2:B:791:SER:HB3   | 2:B:792:LEU:HD23  | 1.81                     | 0.62              |
| 13:M:33:LEU:CD1   | 13:M:36:PRO:HB3   | 2.29                     | 0.62              |
| 1:A:21:SER:HB3    | 1:A:24:GLU:HG2    | 1.81                     | 0.62              |
| 6:H:39:LEU:HD13   | 6:H:125:LEU:HD13  | 1.80                     | 0.62              |
| 1:A:408:LYS:HZ3   | 1:A:409:LEU:HD21  | 1.59                     | 0.62              |
| 2:B:216:ARG:HB2   | 2:B:334:ILE:CG2   | 2.26                     | 0.62              |
| 11:N:146:ARG:HH12 | 11:N:148:ARG:NH2  | 1.92                     | 0.62              |
| 2:B:146:CYS:SG    | 2:B:147:ASN:N     | 2.73                     | 0.62              |
| 2:B:743:VAL:HG22  | 2:B:913:ILE:HB    | 1.81                     | 0.62              |
| 2:B:936:LYS:HE3   | 2:B:966:LEU:CD2   | 2.29                     | 0.62              |
| 9:K:55:LEU:HD21   | 9:K:96:PHE:CE1    | 2.34                     | 0.62              |
| 1:A:122:CYS:SG    | 1:A:165:THR:HG21  | 2.40                     | 0.62              |
| 1:A:1681:LEU:HD21 | 2:B:1123:LEU:HD21 | 1.81                     | 0.62              |
| 2:B:113:LYS:HG3   | 2:B:133:PHE:HE1   | 1.65                     | 0.62              |
| 2:B:570:LEU:HD11  | 11:N:83:LEU:HD11  | 1.80                     | 0.62              |
| 8:J:1:MET:HE2     | 8:J:56:ILE:HD13   | 1.80                     | 0.62              |
| 11:N:142:PRO:HG2  | 11:N:145:LEU:HD21 | 0.70                     | 0.62              |
| 1:A:607:GLU:HB3   | 2:B:1050:THR:HG22 | 1.82                     | 0.62              |
| 1:A:1223:SER:HB2  | 1:A:1245:ILE:CD1  | 2.29                     | 0.62              |
| 1:A:1338:ILE:HG23 | 1:A:1339:LEU:HD12 | 1.81                     | 0.62              |
| 2:B:146:CYS:O     | 2:B:149:ARG:HG2   | 1.99                     | 0.62              |
| 6:H:39:LEU:CD1    | 6:H:125:LEU:HD13  | 2.28                     | 0.62              |
| 15:T:-7:DG:H2'    | 15:T:-6:DA:H1'    | 1.81                     | 0.62              |
| 1:A:846:TRP:HE1   | 1:A:858:PHE:HE1   | 1.48                     | 0.62              |
| 2:B:742:ILE:HD13  | 2:B:996:VAL:HG22  | 1.81                     | 0.62              |
| 2:B:568:LYS:HE2   | 2:B:600:MET:CE    | 2.29                     | 0.62              |
| 2:B:647:PHE:O     | 2:B:650:GLU:HB2   | 1.99                     | 0.62              |
| 2:B:936:LYS:HE3   | 2:B:966:LEU:HD22  | 1.80                     | 0.62              |
| 1:A:127:LEU:HD21  | 1:A:135:VAL:CG2   | 2.30                     | 0.62              |
| 1:A:1335:PRO:HA   | 1:A:1338:ILE:HG22 | 1.82                     | 0.62              |
| 1:A:1583:ILE:HD11 | 1:A:1607:ALA:CB   | 2.30                     | 0.62              |
| 2:B:695:THR:HG21  | 2:B:737:ILE:HG12  | 1.81                     | 0.62              |
| 2:B:791:SER:HA    | 2:B:830:ASN:HA    | 1.81                     | 0.62              |
| 13:M:67:LEU:CD2   | 13:M:69:TYR:CE1   | 2.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:223:LEU:O     | 1:A:256:LEU:HB2   | 2.00                     | 0.61              |
| 1:A:225:ILE:HG23  | 1:A:256:LEU:CD1   | 2.30                     | 0.61              |
| 1:A:423:LYS:HG3   | 1:A:424:LYS:H     | 1.63                     | 0.61              |
| 1:A:1004:ASP:OD1  | 1:A:1006:THR:HG22 | 2.01                     | 0.61              |
| 2:B:583:VAL:HG13  | 2:B:630:LYS:HB3   | 1.81                     | 0.61              |
| 9:K:25:THR:HB     | 9:K:46:GLU:OE1    | 2.00                     | 0.61              |
| 2:B:237:ASN:HD21  | 2:B:244:LEU:HD22  | 1.65                     | 0.61              |
| 10:L:16:ILE:HG23  | 10:L:25:GLU:HB3   | 1.81                     | 0.61              |
| 3:C:241:LEU:HD23  | 3:C:297:VAL:HG22  | 1.80                     | 0.61              |
| 3:C:326:ILE:HG21  | 9:K:111:LEU:HB2   | 1.82                     | 0.61              |
| 1:A:790:GLN:NE2   | 2:B:983:ILE:HD13  | 2.15                     | 0.61              |
| 1:A:1024:LEU:HD12 | 1:A:1204:LEU:HD12 | 1.81                     | 0.61              |
| 1:A:1569:ASN:O    | 1:A:1573:GLU:HA   | 2.00                     | 0.61              |
| 2:B:791:SER:HA    | 2:B:830:ASN:OD1   | 2.00                     | 0.61              |
| 3:C:33:TYR:CB     | 3:C:36:TYR:HB3    | 2.29                     | 0.61              |
| 4:E:173:ILE:HG23  | 4:E:209:VAL:HA    | 1.81                     | 0.61              |
| 1:A:408:LYS:NZ    | 1:A:409:LEU:HD21  | 2.12                     | 0.61              |
| 1:A:137:GLU:OE1   | 1:A:140:ARG:NH2   | 2.34                     | 0.61              |
| 1:A:1498:MET:HA   | 1:A:1501:ARG:HH12 | 1.65                     | 0.61              |
| 1:A:1670:GLN:O    | 1:A:1671:GLN:HB3  | 2.00                     | 0.61              |
| 2:B:752:ASP:O     | 2:B:916:ASN:HB2   | 2.00                     | 0.61              |
| 1:A:1282:LYS:CE   | 1:A:1564:LEU:HD13 | 2.27                     | 0.61              |
| 2:B:92:ILE:HG22   | 2:B:93:CYS:N      | 2.16                     | 0.61              |
| 11:N:61:VAL:HG11  | 13:M:11:TRP:CE3   | 2.35                     | 0.61              |
| 1:A:549:LEU:HD11  | 2:B:1053:LEU:HD13 | 1.81                     | 0.61              |
| 1:A:970:ALA:O     | 1:A:973:GLU:HG2   | 2.00                     | 0.61              |
| 1:A:1289:CYS:N    | 1:A:1292:GLU:OE2  | 2.31                     | 0.61              |
| 2:B:680:ASN:HD21  | 2:B:887:HIS:HD2   | 1.46                     | 0.61              |
| 3:C:12:SER:O      | 3:C:303:ARG:N     | 2.34                     | 0.61              |
| 4:E:126:ILE:O     | 4:E:126:ILE:HG13  | 1.99                     | 0.61              |
| 1:A:812:ARG:HG3   | 1:A:876:ILE:HG23  | 1.82                     | 0.61              |
| 1:A:895:GLN:O     | 1:A:896:MET:HB3   | 2.01                     | 0.61              |
| 1:A:664:LYS:N     | 1:A:664:LYS:HD2   | 2.16                     | 0.60              |
| 2:B:312:LEU:HD21  | 2:B:327:LEU:HD12  | 1.82                     | 0.60              |
| 3:C:18:GLU:HB2    | 3:C:288:PHE:CD2   | 2.36                     | 0.60              |
| 3:C:264:VAL:HG13  | 3:C:264:VAL:O     | 2.00                     | 0.60              |
| 6:H:63:THR:HA     | 6:H:71:ASP:OD1    | 2.01                     | 0.60              |
| 3:C:30:PRO:CG     | 9:K:61:LYS:HA     | 2.31                     | 0.60              |
| 1:A:37:ARG:HH11   | 1:A:40:ASP:HA     | 1.67                     | 0.60              |
| 1:A:919:ILE:HG12  | 1:A:949:GLY:O     | 2.01                     | 0.60              |
| 1:A:926:PRO:HD2   | 1:A:948:GLY:O     | 2.01                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:37:LEU:O      | 4:E:41:LYS:HG2    | 2.01                     | 0.60              |
| 2:B:703:TYR:HE1   | 2:B:711:LEU:HD22  | 1.67                     | 0.60              |
| 8:J:40:LEU:CD1    | 8:J:49:LEU:HD12   | 2.31                     | 0.60              |
| 1:A:132:LEU:HG    | 4:E:210:GLN:NE2   | 2.10                     | 0.60              |
| 2:B:568:LYS:HG3   | 2:B:600:MET:HE2   | 1.84                     | 0.60              |
| 9:K:22:GLU:HG2    | 9:K:25:THR:OG1    | 2.02                     | 0.60              |
| 9:K:83:ARG:HH11   | 9:K:85:GLN:HE21   | 1.48                     | 0.60              |
| 1:A:468:TYR:CE2   | 1:A:605:ARG:HD2   | 2.37                     | 0.60              |
| 1:A:1037:PHE:N    | 1:A:1038:PRO:HD2  | 2.16                     | 0.60              |
| 1:A:1170:TYR:HE2  | 1:A:1192:LEU:HD21 | 1.67                     | 0.60              |
| 1:A:1541:SER:HA   | 1:A:1544:VAL:HG22 | 1.83                     | 0.60              |
| 2:B:185:PRO:O     | 2:B:372:GLN:HA    | 2.01                     | 0.60              |
| 3:C:337:LEU:HD12  | 9:K:104:MET:CE    | 2.32                     | 0.60              |
| 7:I:36:VAL:O      | 7:I:36:VAL:HG12   | 2.02                     | 0.60              |
| 2:B:201:ARG:HB2   | 2:B:205:TYR:HD2   | 1.67                     | 0.60              |
| 1:A:1523:LEU:HD12 | 1:A:1524:TRP:N    | 2.17                     | 0.60              |
| 3:C:245:VAL:HG21  | 3:C:253:LEU:CD2   | 2.32                     | 0.60              |
| 2:B:498:CYS:HB2   | 2:B:668:SER:HB2   | 1.84                     | 0.59              |
| 2:B:758:ILE:HD13  | 2:B:895:ARG:HB2   | 1.84                     | 0.59              |
| 2:B:1067:ALA:HB2  | 2:B:1117:ARG:NE   | 2.16                     | 0.59              |
| 2:B:1068:HIS:CB   | 2:B:1109:THR:HA   | 2.31                     | 0.59              |
| 1:A:951:VAL:HG22  | 1:A:963:GLU:OE1   | 2.01                     | 0.59              |
| 2:B:526:TYR:CE2   | 2:B:528:ALA:HB3   | 2.37                     | 0.59              |
| 2:B:403:LYS:HB2   | 2:B:418:ARG:NH1   | 2.14                     | 0.59              |
| 6:H:14:ASP:HB2    | 6:H:29:HIS:HB2    | 1.85                     | 0.59              |
| 1:A:502:GLY:O     | 1:A:503:SER:OG    | 2.18                     | 0.59              |
| 6:H:100:GLU:HG3   | 6:H:100:GLU:O     | 2.02                     | 0.59              |
| 1:A:866:LYS:HA    | 1:A:869:VAL:HG22  | 1.84                     | 0.59              |
| 1:A:898:VAL:HG21  | 1:A:909:THR:HG21  | 1.83                     | 0.59              |
| 1:A:1505:VAL:HG22 | 1:A:1509:HIS:CE1  | 2.38                     | 0.59              |
| 1:A:1669:LEU:HB2  | 1:A:1691:ASP:OD2  | 2.03                     | 0.59              |
| 2:B:75:PHE:CE2    | 2:B:397:LYS:HE3   | 2.37                     | 0.59              |
| 2:B:1026:ILE:HG22 | 2:B:1033:GLY:HA2  | 1.84                     | 0.59              |
| 1:A:404:SER:O     | 1:A:413:LYS:HD2   | 2.03                     | 0.59              |
| 1:A:408:LYS:HZ1   | 1:A:409:LEU:CD2   | 2.15                     | 0.59              |
| 1:A:1006:THR:HG23 | 1:A:1008:ARG:HG3  | 1.83                     | 0.59              |
| 1:A:1565:ASN:HD22 | 1:A:1579:ASN:ND2  | 2.01                     | 0.59              |
| 3:C:93:LEU:HD22   | 10:L:54:VAL:HG22  | 1.84                     | 0.59              |
| 6:H:24:ARG:HG2    | 6:H:46:GLN:OE1    | 2.02                     | 0.59              |
| 9:K:44:LEU:HD12   | 9:K:80:ILE:HD11   | 1.84                     | 0.59              |
| 1:A:1117:THR:O    | 1:A:1121:LEU:HD23 | 2.03                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:39:THR:HG22  | 2:B:469:PHE:CG    | 2.38                     | 0.59              |
| 2:B:229:LEU:HD21 | 2:B:235:MET:HB2   | 1.85                     | 0.59              |
| 2:B:1030:ASN:OD1 | 2:B:1031:VAL:N    | 2.35                     | 0.59              |
| 9:K:66:GLU:HB3   | 9:K:87:ARG:HE     | 1.67                     | 0.59              |
| 2:B:64:PHE:CE2   | 2:B:397:LYS:HB2   | 2.35                     | 0.58              |
| 2:B:106:ARG:HG2  | 2:B:855:CYS:HB3   | 1.84                     | 0.58              |
| 2:B:536:ASN:OD1  | 11:N:48:PRO:HB3   | 2.03                     | 0.58              |
| 3:C:42:GLN:O     | 3:C:46:GLU:HG3    | 2.03                     | 0.58              |
| 3:C:290:ASN:ND2  | 3:C:293:LEU:HD12  | 2.18                     | 0.58              |
| 1:A:122:CYS:HB3  | 1:A:165:THR:CG2   | 2.31                     | 0.58              |
| 1:A:521:GLN:HA   | 1:A:524:THR:CB    | 2.23                     | 0.58              |
| 1:A:603:LEU:HD22 | 2:B:1052:PHE:CD2  | 2.39                     | 0.58              |
| 2:B:68:PHE:HB3   | 2:B:73:ILE:HD11   | 1.83                     | 0.58              |
| 2:B:753:MET:HA   | 2:B:916:ASN:HD22  | 1.68                     | 0.58              |
| 2:B:882:LYS:HD2  | 2:B:1002:LEU:HD23 | 1.85                     | 0.58              |
| 1:A:39:LEU:HD12  | 1:A:39:LEU:O      | 2.03                     | 0.58              |
| 2:B:239:ILE:HD11 | 2:B:242:LYS:HA    | 1.85                     | 0.58              |
| 2:B:416:LEU:HA   | 2:B:419:ILE:HG12  | 1.85                     | 0.58              |
| 2:B:648:GLU:O    | 2:B:649:ASP:HB2   | 2.03                     | 0.58              |
| 4:E:60:VAL:HG22  | 4:E:74:VAL:HB     | 1.84                     | 0.58              |
| 1:A:91:LEU:H     | 1:A:91:LEU:HD23   | 1.69                     | 0.58              |
| 1:A:112:CYS:HB2  | 1:A:117:ILE:HD11  | 1.85                     | 0.58              |
| 1:A:435:LYS:HD2  | 2:B:1058:LEU:O    | 2.03                     | 0.58              |
| 1:A:1145:PRO:HG2 | 4:E:202:ARG:O     | 2.03                     | 0.58              |
| 2:B:139:ILE:HG22 | 2:B:140:MET:O     | 2.02                     | 0.58              |
| 3:C:30:PRO:HG2   | 9:K:60:MET:O      | 2.03                     | 0.58              |
| 3:C:91:LYS:HE2   | 10:L:54:VAL:CG1   | 2.32                     | 0.58              |
| 13:M:68:SER:O    | 13:M:111:PRO:HA   | 2.02                     | 0.58              |
| 4:E:35:GLN:HA    | 4:E:39:GLU:OE2    | 2.03                     | 0.58              |
| 13:M:11:TRP:CE2  | 13:M:101:VAL:HG21 | 2.39                     | 0.58              |
| 15:T:6:DA:H2'    | 15:T:7:DG:C8      | 2.38                     | 0.58              |
| 1:A:553:GLN:HG2  | 15:T:3:DG:C4'     | 2.33                     | 0.58              |
| 1:A:1110:ARG:HB3 | 1:A:1118:GLN:HE22 | 1.69                     | 0.58              |
| 2:B:549:SER:O    | 2:B:550:TYR:HB2   | 2.02                     | 0.58              |
| 2:B:703:TYR:HE1  | 2:B:711:LEU:CD2   | 2.17                     | 0.58              |
| 1:A:33:ILE:CD1   | 1:A:50:LEU:HD13   | 2.34                     | 0.58              |
| 1:A:93:PHE:CZ    | 1:A:223:LEU:HD11  | 2.39                     | 0.58              |
| 1:A:438:ASP:HB3  | 2:B:1014:THR:O    | 2.04                     | 0.58              |
| 1:A:797:LEU:HD12 | 1:A:897:MET:CE    | 2.34                     | 0.58              |
| 2:B:92:ILE:HD11  | 2:B:858:ASP:O     | 2.03                     | 0.58              |
| 2:B:414:ASP:HA   | 2:B:417:MET:HE2   | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:781:LEU:CD2   | 2:B:792:LEU:HB3   | 2.31                     | 0.58              |
| 1:A:754:TYR:CD1   | 1:A:781:LEU:HD13  | 2.37                     | 0.58              |
| 1:A:718:LYS:HG3   | 6:H:21:LYS:HB2    | 1.85                     | 0.57              |
| 2:B:66:PHE:HZ     | 2:B:400:PHE:CD2   | 2.21                     | 0.57              |
| 2:B:130:ILE:HG21  | 2:B:419:ILE:HD13  | 1.86                     | 0.57              |
| 2:B:743:VAL:CG2   | 2:B:999:TYR:HE2   | 2.16                     | 0.57              |
| 3:C:245:VAL:HG23  | 3:C:273:ALA:HB3   | 1.85                     | 0.57              |
| 1:A:488:PRO:HG3   | 1:A:508:SER:HA    | 1.86                     | 0.57              |
| 1:A:652:HIS:O     | 1:A:656:LEU:HB2   | 2.04                     | 0.57              |
| 3:C:86:THR:CG2    | 3:C:227:PRO:HB3   | 2.34                     | 0.57              |
| 6:H:103:GLU:OE1   | 6:H:103:GLU:N     | 2.29                     | 0.57              |
| 13:M:72:ASN:ND2   | 13:M:74:PHE:O     | 2.37                     | 0.57              |
| 1:A:1318:ARG:HA   | 1:A:1526:GLN:HA   | 1.86                     | 0.57              |
| 2:B:524:PHE:CE2   | 2:B:616:PRO:HG3   | 2.39                     | 0.57              |
| 3:C:245:VAL:CG1   | 3:C:296:VAL:HG11  | 2.35                     | 0.57              |
| 1:A:84:PRO:HD3    | 1:A:335:VAL:HG22  | 1.85                     | 0.57              |
| 1:A:677:LYS:O     | 1:A:678:PRO:C     | 2.42                     | 0.57              |
| 2:B:554:TYR:O     | 2:B:565:TRP:HA    | 2.05                     | 0.57              |
| 4:E:73:PHE:HB2    | 4:E:99:ILE:CD1    | 2.34                     | 0.57              |
| 1:A:137:GLU:HG2   | 1:A:164:TYR:CZ    | 2.39                     | 0.57              |
| 2:B:392:TRP:HE1   | 2:B:423:GLY:CA    | 2.13                     | 0.57              |
| 1:A:654:MET:O     | 1:A:655:GLU:HB3   | 2.05                     | 0.57              |
| 1:A:739:ILE:HD13  | 1:A:761:LEU:HD13  | 1.87                     | 0.57              |
| 1:A:873:SER:HB2   | 1:A:915:LEU:CD2   | 2.34                     | 0.57              |
| 2:B:889:GLN:NE2   | 2:B:925:THR:OG1   | 2.36                     | 0.57              |
| 4:E:122:ALA:HB1   | 4:E:123:PRO:HD2   | 1.85                     | 0.57              |
| 6:H:147:LYS:O     | 6:H:148:LEU:HD23  | 2.04                     | 0.57              |
| 1:A:76:GLY:HA3    | 1:A:306:PRO:HB3   | 1.86                     | 0.57              |
| 2:B:141:VAL:HG12  | 2:B:142:LYS:HG2   | 1.87                     | 0.57              |
| 2:B:201:ARG:HB2   | 2:B:205:TYR:CD2   | 2.40                     | 0.57              |
| 2:B:821:TYR:HB2   | 2:B:844:LYS:NZ    | 2.18                     | 0.57              |
| 2:B:854:VAL:HG12  | 10:L:34:ILE:HG21  | 1.87                     | 0.57              |
| 1:A:42:LEU:O      | 1:A:42:LEU:HD23   | 2.04                     | 0.57              |
| 1:A:225:ILE:HG23  | 1:A:256:LEU:HG    | 1.85                     | 0.57              |
| 1:A:1533:LEU:H    | 1:A:1535:LYS:HZ2  | 1.51                     | 0.57              |
| 2:B:186:ARG:HG3   | 2:B:187:ARG:H     | 1.69                     | 0.57              |
| 11:N:70:LYS:HE2   | 11:N:79:ARG:CZ    | 2.34                     | 0.57              |
| 1:A:1117:THR:HG22 | 1:A:1121:LEU:HD23 | 1.85                     | 0.57              |
| 1:A:1585:LEU:HB2  | 1:A:1586:PRO:HD3  | 1.87                     | 0.57              |
| 2:B:742:ILE:CD1   | 2:B:996:VAL:HG22  | 2.34                     | 0.57              |
| 3:C:75:ALA:HA     | 9:K:50:THR:HG23   | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:I:9:THR:CG2     | 7:I:15:SER:HA     | 2.34                     | 0.57              |
| 1:A:749:LEU:HD23  | 1:A:754:TYR:CE2   | 2.39                     | 0.57              |
| 1:A:1110:ARG:HB3  | 1:A:1118:GLN:NE2  | 2.19                     | 0.57              |
| 1:A:1585:LEU:HD12 | 1:A:1600:LEU:HD21 | 1.87                     | 0.57              |
| 2:B:700:LEU:HD21  | 2:B:711:LEU:HD11  | 1.86                     | 0.57              |
| 2:B:745:VAL:HG12  | 2:B:917:PRO:HB3   | 1.86                     | 0.57              |
| 4:E:165:LEU:HD23  | 4:E:169:GLN:HE21  | 1.68                     | 0.57              |
| 11:N:49:ALA:HA    | 13:M:86:ARG:HG3   | 1.87                     | 0.57              |
| 2:B:600:MET:HB3   | 2:B:608:PRO:CB    | 2.32                     | 0.56              |
| 3:C:98:THR:O      | 3:C:206:GLN:HG2   | 2.05                     | 0.56              |
| 11:N:45:ILE:HB    | 13:M:88:PHE:HB2   | 1.87                     | 0.56              |
| 1:A:430:LYS:HA    | 2:B:1036:ARG:HH21 | 1.70                     | 0.56              |
| 1:A:1631:VAL:HG23 | 1:A:1632:TYR:CD2  | 2.39                     | 0.56              |
| 2:B:527:THR:OG1   | 2:B:530:ILE:HD12  | 2.05                     | 0.56              |
| 4:E:142:HIS:HB3   | 4:E:145:VAL:HG23  | 1.85                     | 0.56              |
| 13:M:11:TRP:CZ2   | 13:M:101:VAL:HG21 | 2.40                     | 0.56              |
| 1:A:507:LEU:CD2   | 1:A:518:VAL:HG11  | 2.35                     | 0.56              |
| 1:A:674:SER:HB3   | 1:A:686:GLN:OE1   | 2.05                     | 0.56              |
| 1:A:1618:LEU:HD11 | 1:A:1649:CYS:HB2  | 1.87                     | 0.56              |
| 2:B:1028:GLY:H    | 2:B:1033:GLY:HA3  | 1.70                     | 0.56              |
| 8:J:63:ALA:HB1    | 10:L:23:HIS:NE2   | 2.20                     | 0.56              |
| 1:A:553:GLN:HG2   | 15:T:3:DG:H4'     | 1.86                     | 0.56              |
| 1:A:1531:LEU:HB3  | 1:A:1535:LYS:CD   | 2.36                     | 0.56              |
| 6:H:36:LYS:HA     | 6:H:36:LYS:HE3    | 1.87                     | 0.56              |
| 1:A:438:ASP:OD1   | 2:B:1025:PRO:HG3  | 2.06                     | 0.56              |
| 2:B:333:CYS:HB3   | 2:B:342:LYS:HG3   | 1.88                     | 0.56              |
| 2:B:696:MET:HG3   | 2:B:712:TYR:HB3   | 1.87                     | 0.56              |
| 7:I:13:PHE:CE1    | 7:I:20:CYS:HB3    | 2.41                     | 0.56              |
| 2:B:781:LEU:HD23  | 2:B:792:LEU:HD22  | 1.85                     | 0.56              |
| 4:E:80:PRO:O      | 4:E:108:GLN:HB2   | 2.05                     | 0.56              |
| 1:A:225:ILE:HG23  | 1:A:256:LEU:HD11  | 1.88                     | 0.56              |
| 1:A:1213:LEU:HD22 | 2:B:1046:LEU:CD1  | 2.35                     | 0.56              |
| 1:A:1318:ARG:CD   | 1:A:1524:TRP:HE3  | 2.18                     | 0.56              |
| 2:B:530:ILE:HB    | 2:B:531:PRO:HD3   | 1.87                     | 0.56              |
| 2:B:736:PRO:HG2   | 8:J:53:VAL:HG11   | 1.87                     | 0.56              |
| 10:L:19:CYS:HB3   | 10:L:23:HIS:H     | 1.71                     | 0.56              |
| 1:A:505:THR:HG23  | 1:A:505:THR:O     | 2.06                     | 0.56              |
| 1:A:914:CYS:O     | 1:A:915:LEU:HB2   | 2.05                     | 0.56              |
| 1:A:1083:LEU:HD12 | 1:A:1083:LEU:O    | 2.06                     | 0.56              |
| 1:A:1502:VAL:O    | 1:A:1505:VAL:HG12 | 2.06                     | 0.56              |
| 2:B:785:ILE:HD12  | 2:B:791:SER:HB2   | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:827:VAL:HG22  | 1:A:861:ILE:CG2   | 2.36                     | 0.56              |
| 1:A:1090:LEU:HD11 | 4:E:33:LEU:CD1    | 2.36                     | 0.56              |
| 1:A:1239:MET:HG3  | 1:A:1239:MET:O    | 2.05                     | 0.56              |
| 2:B:103:CYS:SG    | 2:B:171:ILE:HG21  | 2.45                     | 0.56              |
| 1:A:8:PRO:O       | 1:A:9:TRP:HB3     | 2.05                     | 0.56              |
| 1:A:921:LEU:HA    | 1:A:973:GLU:OE2   | 2.06                     | 0.56              |
| 1:A:1637:ASP:OD2  | 1:A:1639:ARG:HD3  | 2.06                     | 0.56              |
| 6:H:110:THR:HG23  | 6:H:110:THR:O     | 2.06                     | 0.56              |
| 1:A:1583:ILE:HD12 | 1:A:1604:ASP:HB2  | 1.88                     | 0.55              |
| 2:B:1059:PHE:CE2  | 2:B:1064:ARG:HD3  | 2.40                     | 0.55              |
| 3:C:138:LEU:HD21  | 3:C:190:ILE:HD13  | 1.86                     | 0.55              |
| 1:A:19:MET:HG2    | 1:A:296:VAL:CG1   | 2.37                     | 0.55              |
| 1:A:912:ILE:CD1   | 2:B:924:MET:HG2   | 2.35                     | 0.55              |
| 1:A:961:PRO:HD2   | 1:A:962:PRO:HD2   | 1.89                     | 0.55              |
| 1:A:1128:ASP:HB3  | 1:A:1133:ARG:HD3  | 1.88                     | 0.55              |
| 1:A:1300:GLN:HE21 | 7:I:48:ARG:HH11   | 1.53                     | 0.55              |
| 1:A:1685:THR:HG21 | 2:B:1128:ILE:HG12 | 1.86                     | 0.55              |
| 1:A:619:LEU:HD22  | 1:A:624:GLY:O     | 2.06                     | 0.55              |
| 1:A:972:ARG:NH1   | 2:B:489:LEU:HD12  | 2.22                     | 0.55              |
| 1:A:1213:LEU:O    | 1:A:1217:GLN:HG3  | 2.06                     | 0.55              |
| 3:C:288:PHE:CZ    | 3:C:299:LEU:HD21  | 2.41                     | 0.55              |
| 9:K:89:THR:HG23   | 9:K:90:LEU:N      | 2.20                     | 0.55              |
| 1:A:1512:ILE:HD12 | 1:A:1527:VAL:HG21 | 1.86                     | 0.55              |
| 16:U:4:DT:H2'     | 16:U:5:DC:C6      | 2.41                     | 0.55              |
| 1:A:14:GLY:HA2    | 1:A:1691:ASP:O    | 2.06                     | 0.55              |
| 1:A:123:GLN:O     | 1:A:127:LEU:HD23  | 2.06                     | 0.55              |
| 2:B:61:ILE:HG22   | 2:B:61:ILE:O      | 2.06                     | 0.55              |
| 2:B:1026:ILE:HG21 | 2:B:1031:VAL:CG1  | 2.37                     | 0.55              |
| 2:B:1112:VAL:HG22 | 2:B:1113:PRO:HD2  | 1.88                     | 0.55              |
| 3:C:28:ASP:O      | 3:C:29:PHE:HD1    | 1.89                     | 0.55              |
| 1:A:459:PRO:HB2   | 1:A:572:GLU:O     | 2.06                     | 0.55              |
| 1:A:799:VAL:O     | 1:A:803:LEU:HG    | 2.07                     | 0.55              |
| 1:A:1605:ILE:HG21 | 1:A:1621:ILE:CG1  | 2.36                     | 0.55              |
| 2:B:10:LEU:CD1    | 2:B:11:PRO:HD2    | 2.30                     | 0.55              |
| 2:B:86:THR:HG23   | 2:B:96:ALA:O      | 2.05                     | 0.55              |
| 2:B:399:ALA:O     | 2:B:418:ARG:NH1   | 2.39                     | 0.55              |
| 3:C:183:ASP:O     | 3:C:184:LEU:HB3   | 2.06                     | 0.55              |
| 1:A:711:ILE:N     | 1:A:750:ASP:OD2   | 2.35                     | 0.55              |
| 1:A:1693:LEU:HD13 | 1:A:1702:VAL:HG21 | 1.88                     | 0.55              |
| 1:A:1714:GLU:HG2  | 5:F:109:TYR:HE2   | 1.72                     | 0.55              |
| 3:C:74:ASN:O      | 3:C:78:ARG:HG3    | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:M:68:SER:HB2   | 13:M:112:LEU:CB   | 2.36                     | 0.55              |
| 1:A:1293:VAL:HA   | 1:A:1322:LEU:HD12 | 1.87                     | 0.55              |
| 4:E:54:ARG:HD2    | 4:E:57:ASP:CB     | 2.35                     | 0.55              |
| 6:H:104:THR:HB    | 6:H:109:ALA:CB    | 2.37                     | 0.55              |
| 11:N:142:PRO:HG3  | 11:N:145:LEU:HD21 | 1.72                     | 0.55              |
| 1:A:310:ARG:HB3   | 1:A:322:ASN:HD22  | 1.72                     | 0.55              |
| 1:A:651:GLU:CD    | 3:C:29:PHE:HD2    | 2.09                     | 0.55              |
| 2:B:113:LYS:HG3   | 2:B:133:PHE:CE1   | 2.42                     | 0.55              |
| 2:B:903:PRO:HB2   | 2:B:979:LEU:HD23  | 1.89                     | 0.55              |
| 4:E:122:ALA:HB1   | 4:E:123:PRO:CD    | 2.37                     | 0.55              |
| 15:T:-7:DG:H2'    | 15:T:-6:DA:C1'    | 2.36                     | 0.55              |
| 1:A:661:LEU:HG    | 1:A:691:LEU:HD12  | 1.89                     | 0.55              |
| 1:A:1034:PRO:O    | 1:A:1035:LYS:HB3  | 2.06                     | 0.55              |
| 1:A:1221:GLU:HB3  | 1:A:1222:PRO:HD3  | 1.89                     | 0.55              |
| 1:A:1516:GLN:CG   | 1:A:1526:GLN:HG3  | 2.36                     | 0.55              |
| 1:A:1529:VAL:HG12 | 1:A:1530:LYS:N    | 2.22                     | 0.55              |
| 2:B:568:LYS:HG3   | 2:B:600:MET:CE    | 2.37                     | 0.55              |
| 4:E:152:THR:HG23  | 4:E:154:GLU:HG2   | 1.89                     | 0.55              |
| 13:M:67:LEU:CD2   | 13:M:69:TYR:OH    | 2.45                     | 0.55              |
| 1:A:606:ALA:O     | 1:A:610:VAL:HG23  | 2.06                     | 0.54              |
| 2:B:319:PRO:HB2   | 2:B:321:GLU:HG2   | 1.89                     | 0.54              |
| 2:B:651:VAL:HG13  | 2:B:656:THR:CG2   | 2.36                     | 0.54              |
| 5:F:61:GLU:O      | 5:F:65:VAL:HG23   | 2.07                     | 0.54              |
| 7:I:54:VAL:HG12   | 7:I:55:VAL:H      | 1.72                     | 0.54              |
| 11:N:83:LEU:HD12  | 11:N:116:ARG:NH1  | 2.22                     | 0.54              |
| 1:A:10:ARG:HD2    | 2:B:1108:ASP:HB3  | 1.87                     | 0.54              |
| 1:A:220:ASN:O     | 1:A:221:SER:HB2   | 2.07                     | 0.54              |
| 1:A:422:GLU:O     | 1:A:423:LYS:HB2   | 2.08                     | 0.54              |
| 1:A:739:ILE:CD1   | 1:A:761:LEU:HD13  | 2.37                     | 0.54              |
| 1:A:1605:ILE:HG12 | 1:A:1620:VAL:HG12 | 1.89                     | 0.54              |
| 2:B:66:PHE:HE1    | 2:B:75:PHE:CE2    | 2.24                     | 0.54              |
| 7:I:55:VAL:HA     | 7:I:59:VAL:HG11   | 1.89                     | 0.54              |
| 11:N:146:ARG:NH1  | 11:N:148:ARG:HH22 | 1.96                     | 0.54              |
| 1:A:1108:GLU:N    | 1:A:1108:GLU:OE1  | 2.40                     | 0.54              |
| 2:B:194:ILE:HG12  | 2:B:208:TYR:CD1   | 2.42                     | 0.54              |
| 2:B:568:LYS:HE2   | 2:B:600:MET:HE2   | 1.88                     | 0.54              |
| 3:C:15:VAL:HG23   | 3:C:22:ARG:HB2    | 1.89                     | 0.54              |
| 3:C:30:PRO:HA     | 3:C:38:ASP:H      | 1.72                     | 0.54              |
| 3:C:267:VAL:CG1   | 3:C:272:VAL:HG12  | 2.24                     | 0.54              |
| 1:A:312:VAL:CG2   | 1:A:320:PHE:CB    | 2.84                     | 0.54              |
| 2:B:757:MET:HE3   | 2:B:759:VAL:HG23  | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:808:ASP:HB3   | 2:B:814:PHE:CE2   | 2.42                     | 0.54              |
| 9:K:55:LEU:HD23   | 9:K:82:LEU:HD11   | 1.90                     | 0.54              |
| 1:A:522:LEU:O     | 1:A:523:LEU:HB2   | 2.08                     | 0.54              |
| 2:B:1069:VAL:HG21 | 2:B:1134:VAL:HG21 | 1.89                     | 0.54              |
| 3:C:14:VAL:O      | 3:C:300:ALA:HB1   | 2.07                     | 0.54              |
| 4:E:61:LEU:HD12   | 4:E:72:MET:O      | 2.07                     | 0.54              |
| 9:K:86:THR:HG22   | 9:K:92:ALA:HB2    | 1.89                     | 0.54              |
| 1:A:8:PRO:HG2     | 2:B:1111:SER:HB3  | 1.89                     | 0.54              |
| 1:A:654:MET:HE1   | 9:K:60:MET:HE1    | 1.89                     | 0.54              |
| 1:A:1068:HIS:CE1  | 1:A:1144:ASP:O    | 2.61                     | 0.54              |
| 2:B:259:PHE:HA    | 13:M:110:GLN:HE22 | 1.73                     | 0.54              |
| 1:A:121:LEU:O     | 1:A:125:ARG:HG3   | 2.07                     | 0.54              |
| 2:B:703:TYR:O     | 2:B:704:GLN:HB3   | 2.08                     | 0.54              |
| 1:A:905:SER:OG    | 1:A:907:VAL:HG12  | 2.08                     | 0.54              |
| 1:A:1044:TYR:HD1  | 1:A:1195:LEU:HD22 | 1.73                     | 0.54              |
| 2:B:178:VAL:O     | 2:B:178:VAL:HG13  | 2.07                     | 0.54              |
| 2:B:940:LEU:HD23  | 2:B:969:ALA:CB    | 2.37                     | 0.54              |
| 3:C:239:ILE:HD13  | 3:C:261:VAL:HG11  | 1.90                     | 0.54              |
| 7:I:48:ARG:HD3    | 7:I:50:PHE:CZ     | 2.43                     | 0.54              |
| 3:C:13:ARG:HA     | 3:C:301:ARG:O     | 2.08                     | 0.54              |
| 2:B:217:GLU:HB2   | 2:B:219:HIS:CE1   | 2.43                     | 0.53              |
| 2:B:835:GLU:HG3   | 2:B:837:PHE:CZ    | 2.43                     | 0.53              |
| 3:C:12:SER:O      | 3:C:303:ARG:HB2   | 2.08                     | 0.53              |
| 1:A:404:SER:HB2   | 1:A:416:GLY:H     | 1.73                     | 0.53              |
| 1:A:1170:TYR:CE2  | 1:A:1192:LEU:HD21 | 2.42                     | 0.53              |
| 1:A:1300:GLN:NE2  | 7:I:48:ARG:HH11   | 2.06                     | 0.53              |
| 1:A:1714:GLU:HB2  | 5:F:107:ARG:HB3   | 1.89                     | 0.53              |
| 3:C:184:LEU:CD2   | 3:C:185:PHE:CE2   | 2.91                     | 0.53              |
| 11:N:95:LEU:HD11  | 13:M:26:VAL:HG11  | 1.89                     | 0.53              |
| 1:A:30:VAL:HB     | 1:A:66:THR:HG21   | 1.90                     | 0.53              |
| 1:A:182:LYS:O     | 1:A:183:ASN:HB2   | 2.09                     | 0.53              |
| 1:A:668:VAL:H     | 9:K:85:GLN:NE2    | 2.04                     | 0.53              |
| 3:C:337:LEU:HD12  | 9:K:104:MET:HE3   | 1.89                     | 0.53              |
| 5:F:125:ILE:HG13  | 5:F:125:ILE:O     | 2.07                     | 0.53              |
| 6:H:8:ASP:HB3     | 6:H:10:PHE:CE1    | 2.44                     | 0.53              |
| 9:K:58:MET:HG3    | 9:K:103:LEU:HB2   | 1.90                     | 0.53              |
| 1:A:120:LEU:O     | 1:A:124:LEU:HD23  | 2.08                     | 0.53              |
| 1:A:632:GLN:HE22  | 2:B:754:GLU:H     | 1.57                     | 0.53              |
| 1:A:1324:HIS:HA   | 1:A:1327:TYR:CE1  | 2.43                     | 0.53              |
| 1:A:1718:PRO:HD2  | 5:F:103:PRO:O     | 2.08                     | 0.53              |
| 2:B:695:THR:CG2   | 2:B:1000:GLN:HB3  | 2.39                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:13:ILE:HD11   | 4:E:132:GLN:HG3   | 1.91                     | 0.53              |
| 13:M:68:SER:HB2   | 13:M:112:LEU:HB3  | 1.90                     | 0.53              |
| 1:A:1640:HIS:O    | 1:A:1644:VAL:HG23 | 2.07                     | 0.53              |
| 3:C:340:LEU:HD23  | 9:K:97:GLN:HB2    | 1.90                     | 0.53              |
| 1:A:105:LEU:HD12  | 1:A:264:HIS:ND1   | 2.24                     | 0.53              |
| 1:A:457:GLY:HA2   | 1:A:567:ARG:O     | 2.09                     | 0.53              |
| 1:A:960:LYS:HB3   | 1:A:961:PRO:CD    | 2.39                     | 0.53              |
| 1:A:1245:ILE:N    | 1:A:1246:PRO:HD2  | 2.24                     | 0.53              |
| 2:B:514:LEU:HD22  | 2:B:518:CYS:SG    | 2.48                     | 0.53              |
| 3:C:68:ILE:HD11   | 3:C:72:ILE:HG21   | 1.91                     | 0.53              |
| 1:A:180:HIS:HB3   | 1:A:1692:GLU:OE2  | 2.08                     | 0.53              |
| 1:A:280:PHE:O     | 1:A:281:SER:OG    | 2.17                     | 0.53              |
| 2:B:270:LYS:HG3   | 2:B:550:TYR:CD2   | 2.44                     | 0.53              |
| 2:B:656:THR:HG22  | 2:B:656:THR:O     | 2.09                     | 0.53              |
| 2:B:659:GLN:HG3   | 2:B:660:GLU:N     | 2.23                     | 0.53              |
| 3:C:173:MET:HG2   | 3:C:212:MET:HE1   | 1.91                     | 0.53              |
| 4:E:173:ILE:CG2   | 4:E:209:VAL:HA    | 2.38                     | 0.53              |
| 7:I:40:ARG:CD     | 7:I:43:PHE:HA     | 2.36                     | 0.53              |
| 1:A:1519:THR:HG23 | 1:A:1520:GLU:CD   | 2.29                     | 0.53              |
| 1:A:1618:LEU:O    | 1:A:1622:GLU:HG3  | 2.09                     | 0.53              |
| 2:B:75:PHE:CG     | 2:B:397:LYS:HE3   | 2.43                     | 0.53              |
| 2:B:162:GLU:C     | 2:B:164:GLU:H     | 2.11                     | 0.53              |
| 2:B:643:ASN:ND2   | 2:B:655:VAL:HG13  | 2.24                     | 0.53              |
| 1:A:914:CYS:H     | 1:A:954:ARG:CD    | 2.20                     | 0.53              |
| 1:A:1619:ARG:HH22 | 4:E:196:PRO:CD    | 2.20                     | 0.53              |
| 2:B:69:LYS:HD3    | 2:B:407:THR:H     | 1.73                     | 0.53              |
| 2:B:716:THR:O     | 2:B:716:THR:HG23  | 2.09                     | 0.53              |
| 2:B:862:GLY:O     | 10:L:33:PRO:HA    | 2.08                     | 0.53              |
| 3:C:18:GLU:OE1    | 3:C:18:GLU:HA     | 2.08                     | 0.53              |
| 2:B:396:ILE:HG13  | 2:B:397:LYS:N     | 2.22                     | 0.53              |
| 2:B:1068:HIS:HB3  | 2:B:1109:THR:HG22 | 1.91                     | 0.53              |
| 4:E:205:THR:HG22  | 4:E:206:TYR:H     | 1.74                     | 0.53              |
| 8:J:53:VAL:HG13   | 8:J:53:VAL:O      | 2.09                     | 0.53              |
| 15:T:-8:DA:H2"    | 15:T:-7:DG:H8     | 1.74                     | 0.53              |
| 1:A:312:VAL:CG2   | 1:A:320:PHE:HA    | 2.39                     | 0.52              |
| 1:A:618:TYR:CE2   | 1:A:626:PRO:HB3   | 2.44                     | 0.52              |
| 2:B:48:TYR:CE1    | 2:B:52:GLU:HG2    | 2.44                     | 0.52              |
| 2:B:104:ARG:O     | 2:B:707:SER:OG    | 2.22                     | 0.52              |
| 3:C:66:VAL:HG22   | 3:C:305:HIS:CE1   | 2.44                     | 0.52              |
| 4:E:20:LEU:HD12   | 4:E:20:LEU:O      | 2.08                     | 0.52              |
| 6:H:29:HIS:CE1    | 6:H:40:ILE:HD12   | 2.45                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:I:44:ASN:OD1    | 7:I:45:ILE:N      | 2.37                     | 0.52              |
| 1:A:15:ILE:HD13   | 2:B:1132:LEU:HB3  | 1.92                     | 0.52              |
| 1:A:465:LYS:HD3   | 2:B:1012:VAL:HB   | 1.92                     | 0.52              |
| 1:A:613:CYS:O     | 1:A:617:GLN:HG2   | 2.09                     | 0.52              |
| 1:A:1518:ASP:HB3  | 1:A:1523:LEU:H    | 1.73                     | 0.52              |
| 9:K:25:THR:HB     | 9:K:46:GLU:CD     | 2.29                     | 0.52              |
| 1:A:712:THR:HG22  | 1:A:714:LYS:H     | 1.73                     | 0.52              |
| 2:B:808:ASP:HB3   | 2:B:814:PHE:CZ    | 2.44                     | 0.52              |
| 3:C:339:GLU:HG2   | 9:K:26:ALA:CB     | 2.39                     | 0.52              |
| 9:K:42:PHE:HE1    | 9:K:84:ILE:HD12   | 1.73                     | 0.52              |
| 1:A:71:PHE:O      | 1:A:72:SER:OG     | 2.21                     | 0.52              |
| 1:A:550:LEU:HD23  | 1:A:594:MET:SD    | 2.49                     | 0.52              |
| 1:A:667:ARG:HH21  | 9:K:38:HIS:HB2    | 1.74                     | 0.52              |
| 1:A:1589:PHE:HA   | 1:A:1597:LEU:HD13 | 1.91                     | 0.52              |
| 1:A:1619:ARG:HH12 | 4:E:196:PRO:HG2   | 1.74                     | 0.52              |
| 2:B:721:LEU:CD2   | 8:J:50:LEU:HD23   | 2.40                     | 0.52              |
| 2:B:1067:ALA:HB2  | 2:B:1117:ARG:CZ   | 2.40                     | 0.52              |
| 3:C:312:SER:HB3   | 3:C:321:LEU:CD1   | 2.39                     | 0.52              |
| 1:A:85:LEU:CD2    | 1:A:391:TRP:HE1   | 2.23                     | 0.52              |
| 2:B:1014:THR:HG23 | 2:B:1015:THR:H    | 1.73                     | 0.52              |
| 7:I:54:VAL:HG12   | 7:I:55:VAL:N      | 2.23                     | 0.52              |
| 1:A:873:SER:HB2   | 1:A:915:LEU:HD21  | 1.91                     | 0.52              |
| 1:A:1518:ASP:OD2  | 1:A:1525:CYS:HB3  | 2.09                     | 0.52              |
| 1:A:1624:GLU:O    | 1:A:1628:VAL:HG23 | 2.09                     | 0.52              |
| 2:B:742:ILE:HD12  | 8:J:43:TYR:HE1    | 1.75                     | 0.52              |
| 1:A:682:TRP:N     | 1:A:682:TRP:CD1   | 2.76                     | 0.52              |
| 1:A:1293:VAL:O    | 1:A:1293:VAL:HG13 | 2.09                     | 0.52              |
| 1:A:1348:LYS:CE   | 1:A:1508:ILE:HB   | 2.40                     | 0.52              |
| 1:A:1349:LEU:HG   | 1:A:1547:LEU:HD21 | 1.91                     | 0.52              |
| 1:A:1349:LEU:HA   | 1:A:1352:GLU:CD   | 2.30                     | 0.52              |
| 1:A:1512:ILE:HD12 | 1:A:1527:VAL:CG2  | 2.39                     | 0.52              |
| 2:B:262:TYR:HD2   | 13:M:30:ASN:HA    | 1.74                     | 0.52              |
| 16:U:5:DC:H2'     | 16:U:6:DC:C6      | 2.44                     | 0.52              |
| 1:A:166:THR:O     | 1:A:170:GLN:HG2   | 2.09                     | 0.52              |
| 1:A:1096:ILE:HA   | 1:A:1120:MET:CE   | 2.40                     | 0.52              |
| 2:B:972:ASN:HA    | 3:C:286:GLU:OE2   | 2.10                     | 0.52              |
| 2:B:1082:GLU:HG3  | 2:B:1095:LYS:O    | 2.08                     | 0.52              |
| 9:K:124:GLN:O     | 9:K:128:ARG:HG2   | 2.09                     | 0.52              |
| 2:B:169:TYR:CE1   | 2:B:176:GLU:HG2   | 2.44                     | 0.52              |
| 7:I:9:THR:HG22    | 7:I:15:SER:HA     | 1.92                     | 0.52              |
| 1:A:766:TYR:HD1   | 1:A:771:GLY:HA2   | 1.75                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:595:VAL:HA    | 2:B:612:LEU:HD23  | 1.91                     | 0.52              |
| 2:B:943:LEU:HD11  | 11:N:142:PRO:HG3  | 1.90                     | 0.52              |
| 1:A:1154:ILE:HG23 | 1:A:1154:ILE:O    | 2.10                     | 0.51              |
| 5:F:121:ASP:OD1   | 5:F:122:GLU:N     | 2.43                     | 0.51              |
| 13:M:67:LEU:HD21  | 13:M:69:TYR:HH    | 1.71                     | 0.51              |
| 6:H:65:TYR:HB3    | 6:H:67:ASP:OD2    | 2.10                     | 0.51              |
| 11:N:121:PRO:HD2  | 11:N:121:PRO:O    | 2.10                     | 0.51              |
| 1:A:225:ILE:HG23  | 1:A:256:LEU:CG    | 2.40                     | 0.51              |
| 1:A:543:LYS:HG3   | 1:A:543:LYS:O     | 2.10                     | 0.51              |
| 1:A:1359:ASN:O    | 1:A:1360:LYS:HD2  | 2.10                     | 0.51              |
| 1:A:312:VAL:CG2   | 1:A:320:PHE:CA    | 2.88                     | 0.51              |
| 1:A:1497:ALA:O    | 1:A:1498:MET:C    | 2.47                     | 0.51              |
| 2:B:473:HIS:HD2   | 2:B:475:GLY:H     | 1.58                     | 0.51              |
| 2:B:648:GLU:HG2   | 2:B:649:ASP:N     | 2.25                     | 0.51              |
| 3:C:221:ASP:OD2   | 10:L:58:ARG:NH2   | 2.40                     | 0.51              |
| 6:H:137:VAL:O     | 6:H:138:ASP:HB2   | 2.09                     | 0.51              |
| 7:I:43:PHE:CE1    | 7:I:46:ASN:HA     | 2.45                     | 0.51              |
| 1:A:163:GLN:O     | 1:A:166:THR:HG22  | 2.11                     | 0.51              |
| 1:A:215:VAL:HG22  | 1:A:225:ILE:HG22  | 1.92                     | 0.51              |
| 1:A:1134:LYS:HA   | 1:A:1134:LYS:HE2  | 1.92                     | 0.51              |
| 1:A:1318:ARG:HH21 | 1:A:1526:GLN:HG2  | 1.75                     | 0.51              |
| 1:A:1353:SER:OG   | 1:A:1543:LEU:HD11 | 2.11                     | 0.51              |
| 2:B:77:ILE:HG12   | 2:B:118:ILE:HG22  | 1.91                     | 0.51              |
| 2:B:411:MET:HE2   | 2:B:411:MET:N     | 2.24                     | 0.51              |
| 2:B:639:GLN:O     | 2:B:639:GLN:HG2   | 2.09                     | 0.51              |
| 3:C:15:VAL:HA     | 3:C:300:ALA:CB    | 2.40                     | 0.51              |
| 2:B:194:ILE:HG12  | 2:B:208:TYR:CE1   | 2.45                     | 0.51              |
| 2:B:624:GLN:NE2   | 2:B:629:GLY:HA2   | 2.26                     | 0.51              |
| 3:C:335:ARG:NH2   | 9:K:25:THR:O      | 2.43                     | 0.51              |
| 1:A:33:ILE:HD11   | 1:A:81:ILE:HG13   | 1.92                     | 0.51              |
| 1:A:551:ASN:HD21  | 2:B:1041:GLU:HG2  | 1.74                     | 0.51              |
| 1:A:961:PRO:CD    | 1:A:962:PRO:HD2   | 2.41                     | 0.51              |
| 1:A:1068:HIS:HE1  | 1:A:1144:ASP:O    | 1.93                     | 0.51              |
| 1:A:1279:LYS:O    | 1:A:1283:LYS:HD3  | 2.11                     | 0.51              |
| 2:B:691:MET:CE    | 2:B:884:ALA:HB1   | 2.41                     | 0.51              |
| 3:C:163:TYR:CD1   | 3:C:166:HIS:HB3   | 2.39                     | 0.51              |
| 1:A:166:THR:HA    | 1:A:169:VAL:CG2   | 2.41                     | 0.51              |
| 1:A:1583:ILE:HD11 | 1:A:1607:ALA:HB3  | 1.93                     | 0.51              |
| 2:B:743:VAL:HG21  | 2:B:999:TYR:CE2   | 2.42                     | 0.51              |
| 4:E:190:VAL:HG22  | 4:E:208:LEU:CD1   | 2.38                     | 0.51              |
| 8:J:1:MET:HE3     | 8:J:56:ILE:HD13   | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:29:PHE:HB3    | 3:C:30:PRO:CD     | 2.41                     | 0.51              |
| 9:K:86:THR:OG1    | 9:K:90:LEU:HD21   | 2.11                     | 0.51              |
| 1:A:123:GLN:O     | 1:A:126:VAL:HG22  | 2.10                     | 0.51              |
| 1:A:603:LEU:HD22  | 2:B:1052:PHE:CG   | 2.45                     | 0.51              |
| 1:A:841:GLU:O     | 1:A:845:LYS:HG2   | 2.11                     | 0.51              |
| 1:A:601:SER:O     | 1:A:602:GLU:HB3   | 2.10                     | 0.50              |
| 1:A:1147:LEU:HD22 | 1:A:1152:PRO:HB3  | 1.93                     | 0.50              |
| 2:B:785:ILE:HG12  | 2:B:786:LYS:O     | 2.11                     | 0.50              |
| 2:B:920:PHE:N     | 2:B:921:PRO:HD2   | 2.26                     | 0.50              |
| 1:A:163:GLN:HG3   | 1:A:164:TYR:N     | 2.26                     | 0.50              |
| 1:A:428:PHE:O     | 1:A:432:MET:HB3   | 2.11                     | 0.50              |
| 1:A:499:ASN:HD22  | 1:A:536:LYS:HD2   | 1.76                     | 0.50              |
| 1:A:1300:GLN:HB2  | 1:A:1316:GLN:HG2  | 1.94                     | 0.50              |
| 1:A:1625:ILE:HG21 | 1:A:1641:LEU:HD22 | 1.94                     | 0.50              |
| 2:B:419:ILE:HG13  | 2:B:420:PHE:N     | 2.26                     | 0.50              |
| 1:A:465:LYS:O     | 1:A:467:THR:HG23  | 2.12                     | 0.50              |
| 1:A:480:LEU:O     | 1:A:484:VAL:HG12  | 2.11                     | 0.50              |
| 1:A:521:GLN:CA    | 1:A:524:THR:HB    | 2.25                     | 0.50              |
| 1:A:1114:SER:OG   | 1:A:1115:PRO:HD2  | 2.10                     | 0.50              |
| 2:B:87:VAL:HB     | 2:B:92:ILE:HD12   | 1.93                     | 0.50              |
| 2:B:948:THR:O     | 2:B:951:ILE:HG12  | 2.11                     | 0.50              |
| 5:F:104:ILE:O     | 5:F:120:VAL:HG23  | 2.10                     | 0.50              |
| 1:A:87:VAL:HB     | 1:A:395:GLN:NE2   | 2.26                     | 0.50              |
| 1:A:802:ILE:HG22  | 1:A:894:LEU:HD22  | 1.92                     | 0.50              |
| 1:A:1086:ARG:CZ   | 1:A:1086:ARG:HB2  | 2.42                     | 0.50              |
| 1:A:1151:ARG:HG3  | 1:A:1153:ASP:OD1  | 2.11                     | 0.50              |
| 1:A:1632:TYR:HB2  | 1:A:1634:ILE:HD12 | 1.94                     | 0.50              |
| 2:B:102:GLU:O     | 2:B:103:CYS:SG    | 2.68                     | 0.50              |
| 4:E:10:LEU:CD2    | 4:E:58:LEU:HD11   | 2.40                     | 0.50              |
| 5:F:107:ARG:HD2   | 5:F:115:TYR:CG    | 2.46                     | 0.50              |
| 1:A:440:ALA:HB1   | 2:B:1035:ILE:HD11 | 1.92                     | 0.50              |
| 2:B:6:ARG:O       | 2:B:6:ARG:HD3     | 2.12                     | 0.50              |
| 2:B:94:LYS:HG2    | 10:L:39:CYS:HA    | 1.91                     | 0.50              |
| 2:B:140:MET:HE2   | 2:B:168:GLY:HA2   | 1.92                     | 0.50              |
| 2:B:172:ILE:HG12  | 2:B:434:PHE:HB3   | 1.93                     | 0.50              |
| 2:B:552:GLU:O     | 2:B:568:LYS:HB2   | 2.11                     | 0.50              |
| 2:B:657:THR:HG22  | 2:B:658:HIS:ND1   | 2.27                     | 0.50              |
| 2:B:743:VAL:CG2   | 2:B:997:VAL:HG22  | 2.41                     | 0.50              |
| 3:C:114:PRO:HG3   | 8:J:13:ILE:CD1    | 2.41                     | 0.50              |
| 4:E:154:GLU:O     | 4:E:158:GLU:HG3   | 2.11                     | 0.50              |
| 13:M:36:PRO:C     | 13:M:38:ASN:H     | 2.15                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:551:ASN:ND2   | 2:B:1041:GLU:HG2 | 2.26                     | 0.50              |
| 2:B:417:MET:O     | 2:B:421:THR:OG1  | 2.30                     | 0.50              |
| 3:C:15:VAL:HG12   | 3:C:298:ARG:HH21 | 1.77                     | 0.50              |
| 3:C:93:LEU:HB3    | 10:L:52:LEU:HD11 | 1.94                     | 0.50              |
| 1:A:1147:LEU:CD2  | 1:A:1152:PRO:HB3 | 2.42                     | 0.50              |
| 2:B:187:ARG:HD2   | 2:B:615:THR:CB   | 2.40                     | 0.50              |
| 2:B:695:THR:HG21  | 2:B:1000:GLN:HB3 | 1.94                     | 0.50              |
| 6:H:92:MET:HE1    | 6:H:121:LEU:CD1  | 2.42                     | 0.50              |
| 2:B:882:LYS:HD2   | 2:B:1002:LEU:CD2 | 2.41                     | 0.50              |
| 1:A:257:THR:HB    | 1:A:391:TRP:HZ3  | 1.77                     | 0.50              |
| 1:A:425:GLU:CG    | 1:A:426:GLY:H    | 2.24                     | 0.50              |
| 1:A:1014:VAL:HG21 | 4:E:165:LEU:HD21 | 1.94                     | 0.50              |
| 2:B:118:ILE:HD11  | 2:B:419:ILE:HG21 | 1.93                     | 0.50              |
| 1:A:57:PRO:HD3    | 1:A:64:CYS:HB3   | 1.93                     | 0.49              |
| 1:A:636:VAL:HG11  | 1:A:795:PHE:CZ   | 2.47                     | 0.49              |
| 1:A:656:LEU:HD13  | 1:A:792:TYR:HE2  | 1.77                     | 0.49              |
| 1:A:791:LEU:HD22  | 2:B:984:SER:HB3  | 1.94                     | 0.49              |
| 1:A:1545:VAL:HG21 | 7:I:53:LYS:NZ    | 2.28                     | 0.49              |
| 2:B:91:THR:HG22   | 2:B:91:THR:O     | 2.12                     | 0.49              |
| 2:B:802:ARG:HB3   | 2:B:838:VAL:HG21 | 1.94                     | 0.49              |
| 2:B:987:GLU:CD    | 3:C:301:ARG:HE   | 2.15                     | 0.49              |
| 1:A:936:PRO:HG2   | 2:B:494:TRP:CD1  | 2.45                     | 0.49              |
| 2:B:263:GLN:CD    | 13:M:29:SER:HB2  | 2.32                     | 0.49              |
| 2:B:396:ILE:CG2   | 2:B:422:MET:HB2  | 2.33                     | 0.49              |
| 2:B:615:THR:HB    | 2:B:616:PRO:HD2  | 1.94                     | 0.49              |
| 2:B:781:LEU:O     | 2:B:792:LEU:HD22 | 2.13                     | 0.49              |
| 8:J:10:CYS:SG     | 8:J:10:CYS:O     | 2.70                     | 0.49              |
| 16:U:6:DC:H2"     | 16:U:7:DT:H71    | 1.92                     | 0.49              |
| 1:A:322:ASN:HB3   | 1:A:325:THR:HG23 | 1.94                     | 0.49              |
| 1:A:1504:ALA:O    | 1:A:1507:GLU:HB3 | 2.12                     | 0.49              |
| 2:B:319:PRO:HG2   | 2:B:322:GLN:HB2  | 1.93                     | 0.49              |
| 2:B:387:GLU:OE1   | 2:B:445:LEU:HD11 | 2.13                     | 0.49              |
| 2:B:901:ASP:OD1   | 3:C:78:ARG:NH1   | 2.38                     | 0.49              |
| 7:I:7:ALA:HB3     | 13:M:34:GLN:HG3  | 1.94                     | 0.49              |
| 7:I:34:ASP:O      | 7:I:35:THR:OG1   | 2.18                     | 0.49              |
| 1:A:1029:THR:O    | 1:A:1033:GLN:NE2 | 2.41                     | 0.49              |
| 2:B:187:ARG:NH1   | 2:B:616:PRO:HD2  | 2.27                     | 0.49              |
| 2:B:1126:MET:O    | 2:B:1127:ASN:HB2 | 2.12                     | 0.49              |
| 3:C:26:THR:OG1    | 3:C:303:ARG:NE   | 2.45                     | 0.49              |
| 7:I:60:VAL:O      | 7:I:60:VAL:HG12  | 2.10                     | 0.49              |
| 13:M:74:PHE:N     | 13:M:78:ALA:HB2  | 2.27                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:137:GLU:OE1   | 1:A:137:GLU:HA    | 2.12                     | 0.49              |
| 1:A:425:GLU:HG3   | 1:A:426:GLY:N     | 2.24                     | 0.49              |
| 1:A:1022:ASP:HB3  | 4:E:200:ALA:CB    | 2.43                     | 0.49              |
| 1:A:1662:ILE:HD13 | 1:A:1674:PHE:HD2  | 1.78                     | 0.49              |
| 2:B:92:ILE:CD1    | 2:B:859:THR:HA    | 2.40                     | 0.49              |
| 2:B:626:LEU:O     | 2:B:627:ALA:HB3   | 2.12                     | 0.49              |
| 3:C:140:PHE:HE2   | 3:C:214:CYS:HG    | 1.60                     | 0.49              |
| 2:B:315:PRO:O     | 2:B:318:TYR:HB2   | 2.12                     | 0.49              |
| 2:B:497:LEU:HD23  | 2:B:512:ASN:CB    | 2.43                     | 0.49              |
| 2:B:648:GLU:HG2   | 2:B:649:ASP:H     | 1.77                     | 0.49              |
| 2:B:655:VAL:HG12  | 2:B:656:THR:H     | 1.76                     | 0.49              |
| 2:B:752:ASP:HB3   | 2:B:758:ILE:HG12  | 1.95                     | 0.49              |
| 3:C:29:PHE:HB3    | 3:C:30:PRO:HD2    | 1.95                     | 0.49              |
| 7:I:14:GLN:HG2    | 7:I:17:LEU:HD12   | 1.95                     | 0.49              |
| 11:N:11:ARG:O     | 11:N:12:PHE:C     | 2.49                     | 0.49              |
| 1:A:19:MET:HG2    | 1:A:296:VAL:HG11  | 1.93                     | 0.49              |
| 1:A:1213:LEU:HD22 | 2:B:1046:LEU:HD11 | 1.95                     | 0.49              |
| 2:B:583:VAL:CG1   | 2:B:630:LYS:HB3   | 2.43                     | 0.49              |
| 3:C:56:MET:HE2    | 9:K:121:TYR:CD2   | 2.47                     | 0.49              |
| 3:C:110:LEU:HD13  | 3:C:212:MET:SD    | 2.53                     | 0.49              |
| 3:C:340:LEU:O     | 3:C:343:VAL:HG22  | 2.12                     | 0.49              |
| 6:H:39:LEU:HD11   | 6:H:123:MET:SD    | 2.52                     | 0.49              |
| 7:I:17:LEU:HD22   | 7:I:35:THR:HB     | 1.95                     | 0.49              |
| 7:I:19:PHE:CE2    | 7:I:34:ASP:HB2    | 2.48                     | 0.49              |
| 1:A:497:VAL:O     | 1:A:505:THR:HG22  | 2.13                     | 0.49              |
| 1:A:1222:PRO:O    | 1:A:1226:MET:N    | 2.44                     | 0.49              |
| 1:A:1505:VAL:HG11 | 1:A:1515:TYR:CZ   | 2.48                     | 0.49              |
| 2:B:426:LEU:HD23  | 2:B:426:LEU:O     | 2.13                     | 0.49              |
| 3:C:90:GLU:HB2    | 3:C:215:VAL:HG22  | 1.94                     | 0.49              |
| 1:A:990:ARG:O     | 1:A:994:LYS:HG2   | 2.13                     | 0.49              |
| 2:B:539:VAL:HG22  | 2:B:566:VAL:HB    | 1.95                     | 0.49              |
| 4:E:205:THR:HG22  | 4:E:206:TYR:N     | 2.27                     | 0.49              |
| 8:J:3:ILE:HD11    | 8:J:49:LEU:HD23   | 1.95                     | 0.49              |
| 9:K:31:GLN:OE1    | 9:K:37:ARG:HA     | 2.12                     | 0.49              |
| 1:A:25:LEU:O      | 1:A:28:LEU:HB2    | 2.13                     | 0.49              |
| 1:A:47:ALA:O      | 1:A:48:ASN:HB2    | 2.12                     | 0.49              |
| 1:A:127:LEU:HD11  | 1:A:187:SER:OG    | 2.13                     | 0.49              |
| 1:A:717:VAL:HG22  | 6:H:20:LYS:HG2    | 1.95                     | 0.49              |
| 1:A:1281:LEU:HD21 | 1:A:1595:LEU:HD11 | 1.94                     | 0.49              |
| 2:B:269:ILE:HD11  | 2:B:282:VAL:HG21  | 1.95                     | 0.49              |
| 7:I:31:GLY:HA3    | 7:I:36:VAL:HG13   | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:N:30:PHE:HZ    | 13:M:102:TYR:CG   | 2.31                     | 0.49              |
| 11:N:41:GLU:OE1   | 13:M:94:LYS:HD3   | 2.12                     | 0.49              |
| 1:A:9:TRP:CG      | 1:A:9:TRP:O       | 2.66                     | 0.48              |
| 1:A:1016:GLN:NE2  | 1:A:1646:ASP:OD2  | 2.46                     | 0.48              |
| 2:B:568:LYS:HE2   | 2:B:600:MET:HE3   | 1.94                     | 0.48              |
| 1:A:144:ARG:CD    | 4:E:122:ALA:HB2   | 2.43                     | 0.48              |
| 1:A:1024:LEU:HD23 | 1:A:1029:THR:HG22 | 1.95                     | 0.48              |
| 1:A:1088:ALA:O    | 1:A:1091:SER:OG   | 2.20                     | 0.48              |
| 1:A:1566:GLU:H    | 1:A:1566:GLU:CD   | 2.16                     | 0.48              |
| 4:E:189:GLN:O     | 4:E:209:VAL:HG23  | 2.13                     | 0.48              |
| 1:A:915:LEU:HD12  | 1:A:952:THR:HA    | 1.95                     | 0.48              |
| 2:B:926:ILE:O     | 2:B:930:ILE:HG13  | 2.13                     | 0.48              |
| 4:E:123:PRO:HA    | 4:E:126:ILE:CG2   | 2.42                     | 0.48              |
| 1:A:1255:ALA:HB3  | 1:A:1656:PRO:HB3  | 1.94                     | 0.48              |
| 2:B:58:VAL:O      | 2:B:61:ILE:HB     | 2.13                     | 0.48              |
| 4:E:80:PRO:HA     | 4:E:107:GLN:HG3   | 1.95                     | 0.48              |
| 7:I:47:VAL:HG23   | 7:I:47:VAL:O      | 2.14                     | 0.48              |
| 1:A:162:GLU:HA    | 1:A:165:THR:OG1   | 2.13                     | 0.48              |
| 1:A:663:ASP:OD1   | 1:A:664:LYS:N     | 2.46                     | 0.48              |
| 1:A:678:PRO:HB2   | 6:H:47:ILE:HG23   | 1.95                     | 0.48              |
| 1:A:1558:GLY:O    | 1:A:1582:GLY:HA3  | 2.14                     | 0.48              |
| 1:A:1702:VAL:CG2  | 1:A:1704:LYS:HG3  | 2.43                     | 0.48              |
| 2:B:745:VAL:CG1   | 2:B:917:PRO:HB3   | 2.43                     | 0.48              |
| 2:B:1069:VAL:CG2  | 2:B:1134:VAL:HG21 | 2.44                     | 0.48              |
| 3:C:222:HIS:CD2   | 10:L:58:ARG:HD3   | 2.49                     | 0.48              |
| 10:L:19:CYS:SG    | 10:L:20:GLY:N     | 2.86                     | 0.48              |
| 1:A:668:VAL:N     | 9:K:85:GLN:HE22   | 2.05                     | 0.48              |
| 7:I:14:GLN:O      | 7:I:15:SER:HB3    | 2.12                     | 0.48              |
| 1:A:1133:ARG:C    | 1:A:1134:LYS:HE2  | 2.33                     | 0.48              |
| 1:A:1605:ILE:HG21 | 1:A:1621:ILE:HG12 | 1.96                     | 0.48              |
| 2:B:166:MET:O     | 2:B:166:MET:HG2   | 2.14                     | 0.48              |
| 2:B:392:TRP:CE3   | 2:B:393:LEU:HD23  | 2.49                     | 0.48              |
| 2:B:399:ALA:HB2   | 2:B:422:MET:HE2   | 1.95                     | 0.48              |
| 2:B:906:GLU:CD    | 3:C:301:ARG:HH22  | 2.17                     | 0.48              |
| 1:A:163:GLN:HG3   | 1:A:164:TYR:H     | 1.79                     | 0.48              |
| 1:A:960:LYS:HB3   | 1:A:961:PRO:HD2   | 1.96                     | 0.48              |
| 2:B:796:ILE:HD12  | 2:B:809:ASP:H     | 1.77                     | 0.48              |
| 3:C:171:ARG:HG3   | 3:C:195:ASP:HB2   | 1.94                     | 0.48              |
| 4:E:17:ILE:HD11   | 4:E:105:VAL:HG21  | 1.95                     | 0.48              |
| 7:I:35:THR:HG21   | 13:M:113:PHE:CE1  | 2.49                     | 0.48              |
| 13:M:26:VAL:HG12  | 13:M:60:LEU:CD2   | 2.44                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1223:SER:HB2  | 1:A:1245:ILE:HD11 | 1.94                     | 0.48              |
| 1:A:1281:LEU:HD11 | 1:A:1591:TYR:CE2  | 2.48                     | 0.48              |
| 2:B:286:LEU:O     | 2:B:290:MET:HB2   | 2.13                     | 0.48              |
| 2:B:571:ALA:HB3   | 2:B:572:PRO:HD3   | 1.94                     | 0.48              |
| 2:B:905:THR:CG2   | 2:B:909:MET:HB2   | 2.43                     | 0.48              |
| 2:B:981:SER:HB2   | 2:B:988:LEU:HD21  | 1.96                     | 0.48              |
| 3:C:56:MET:HE1    | 9:K:122:LYS:HG3   | 1.95                     | 0.48              |
| 9:K:47:GLU:OE1    | 9:K:47:GLU:HA     | 2.14                     | 0.48              |
| 15:T:-2:DA:H2''   | 15:T:-1:DG:C8     | 2.49                     | 0.48              |
| 1:A:164:TYR:O     | 1:A:168:ILE:HG12  | 2.14                     | 0.48              |
| 1:A:677:LYS:HB3   | 1:A:678:PRO:HD3   | 1.94                     | 0.48              |
| 1:A:1122:ARG:O    | 1:A:1127:LEU:HD13 | 2.14                     | 0.48              |
| 2:B:8:ARG:O       | 2:B:9:ASN:ND2     | 2.47                     | 0.48              |
| 2:B:435:ALA:HB1   | 15:T:9:DA:H5''    | 1.94                     | 0.48              |
| 2:B:681:GLN:HG3   | 2:B:683:PRO:HD2   | 1.96                     | 0.48              |
| 3:C:250:ALA:HB1   | 3:C:273:ALA:HB2   | 1.96                     | 0.48              |
| 1:A:683:THR:HG22  | 1:A:683:THR:O     | 2.12                     | 0.47              |
| 1:A:753:HIS:O     | 1:A:754:TYR:HB2   | 2.14                     | 0.47              |
| 2:B:178:VAL:O     | 2:B:178:VAL:HG22  | 2.14                     | 0.47              |
| 5:F:66:LEU:HD21   | 5:F:97:LEU:HD22   | 1.96                     | 0.47              |
| 7:I:34:ASP:C      | 7:I:35:THR:HG1    | 2.12                     | 0.47              |
| 2:B:178:VAL:O     | 2:B:179:ILE:C     | 2.53                     | 0.47              |
| 2:B:410:SER:HB3   | 2:B:411:MET:HE2   | 1.96                     | 0.47              |
| 2:B:498:CYS:CB    | 2:B:668:SER:HB2   | 2.43                     | 0.47              |
| 2:B:746:ILE:HG22  | 2:B:914:LEU:HD22  | 1.95                     | 0.47              |
| 2:B:785:ILE:HD12  | 2:B:791:SER:CB    | 2.43                     | 0.47              |
| 3:C:162:LEU:HG    | 3:C:204:PRO:HD3   | 1.95                     | 0.47              |
| 3:C:182:ALA:O     | 3:C:185:PHE:O     | 2.32                     | 0.47              |
| 7:I:17:LEU:HD13   | 7:I:35:THR:O      | 2.15                     | 0.47              |
| 1:A:89:ASN:HD21   | 1:A:92:LEU:HD12   | 1.78                     | 0.47              |
| 1:A:423:LYS:HG3   | 1:A:424:LYS:N     | 2.27                     | 0.47              |
| 1:A:1498:MET:HA   | 1:A:1501:ARG:NH1  | 2.29                     | 0.47              |
| 1:A:1527:VAL:HG22 | 1:A:1528:THR:N    | 2.30                     | 0.47              |
| 1:A:1681:LEU:HD21 | 2:B:1123:LEU:CD2  | 2.45                     | 0.47              |
| 2:B:527:THR:HG23  | 2:B:527:THR:O     | 2.14                     | 0.47              |
| 5:F:81:VAL:O      | 5:F:81:VAL:HG22   | 2.14                     | 0.47              |
| 6:H:106:THR:O     | 6:H:106:THR:HG22  | 2.13                     | 0.47              |
| 13:M:36:PRO:C     | 13:M:38:ASN:N     | 2.67                     | 0.47              |
| 1:A:591:GLY:O     | 14:R:-1:U:H4'     | 2.14                     | 0.47              |
| 1:A:1084:LEU:HG   | 1:A:1084:LEU:O    | 2.14                     | 0.47              |
| 2:B:122:VAL:O     | 2:B:123:ASN:HB2   | 2.14                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:179:ILE:HG12 | 2:B:454:CYS:HB2   | 1.96                     | 0.47              |
| 3:C:30:PRO:HG2   | 9:K:61:LYS:HA     | 1.95                     | 0.47              |
| 4:E:139:ILE:HG13 | 4:E:140:THR:N     | 2.28                     | 0.47              |
| 6:H:13:LYS:HE2   | 6:H:13:LYS:HA     | 1.95                     | 0.47              |
| 9:K:55:LEU:HD21  | 9:K:96:PHE:HE1    | 1.76                     | 0.47              |
| 11:N:105:LEU:HB2 | 13:M:41:PHE:HB2   | 1.95                     | 0.47              |
| 16:U:2:DT:H2"    | 16:U:3:DG:C8      | 2.50                     | 0.47              |
| 1:A:100:LEU:HD21 | 1:A:265:LEU:HD22  | 1.96                     | 0.47              |
| 1:A:936:PRO:HG2  | 2:B:494:TRP:CG    | 2.50                     | 0.47              |
| 1:A:1106:GLU:N   | 1:A:1106:GLU:OE2  | 2.48                     | 0.47              |
| 1:A:1287:ARG:HG2 | 1:A:1555:ALA:HB1  | 1.96                     | 0.47              |
| 1:A:1545:VAL:CG2 | 7:I:53:LYS:HE3    | 2.41                     | 0.47              |
| 1:A:1669:LEU:O   | 1:A:1673:THR:HG23 | 2.15                     | 0.47              |
| 2:B:141:VAL:O    | 2:B:146:CYS:CB    | 2.63                     | 0.47              |
| 2:B:743:VAL:HG21 | 2:B:997:VAL:HG22  | 1.97                     | 0.47              |
| 3:C:86:THR:HG21  | 3:C:227:PRO:HB3   | 1.96                     | 0.47              |
| 3:C:245:VAL:HG21 | 3:C:253:LEU:HD23  | 1.97                     | 0.47              |
| 3:C:337:LEU:HD21 | 9:K:100:LEU:HB2   | 1.97                     | 0.47              |
| 1:A:845:LYS:HA   | 1:A:845:LYS:HE2   | 1.97                     | 0.47              |
| 1:A:1332:CYS:O   | 1:A:1332:CYS:SG   | 2.73                     | 0.47              |
| 3:C:33:TYR:HB3   | 3:C:36:TYR:CB     | 2.39                     | 0.47              |
| 13:M:36:PRO:O    | 13:M:38:ASN:N     | 2.47                     | 0.47              |
| 1:A:66:THR:O     | 2:B:1083:LYS:HE3  | 2.14                     | 0.47              |
| 1:A:89:ASN:OD1   | 1:A:92:LEU:HB2    | 2.14                     | 0.47              |
| 1:A:119:LEU:HB2  | 1:A:142:LEU:HD22  | 1.97                     | 0.47              |
| 1:A:173:LEU:O    | 1:A:174:LEU:CB    | 2.63                     | 0.47              |
| 1:A:181:VAL:HG11 | 4:E:166:ARG:HH21  | 1.79                     | 0.47              |
| 1:A:257:THR:HB   | 1:A:391:TRP:CZ3   | 2.50                     | 0.47              |
| 2:B:181:MET:SD   | 2:B:520:VAL:HG21  | 2.55                     | 0.47              |
| 2:B:785:ILE:CG2  | 2:B:792:LEU:CD2   | 2.81                     | 0.47              |
| 3:C:27:THR:O     | 3:C:27:THR:HG22   | 2.14                     | 0.47              |
| 4:E:72:MET:CE    | 4:E:103:LEU:HD12  | 2.45                     | 0.47              |
| 1:A:811:LYS:O    | 1:A:814:ARG:HG2   | 2.15                     | 0.47              |
| 1:A:1110:ARG:HD3 | 1:A:1110:ARG:C    | 2.35                     | 0.47              |
| 1:A:1247:ARG:HG2 | 1:A:1628:VAL:HG22 | 1.97                     | 0.47              |
| 1:A:1253:MET:O   | 1:A:1658:ASN:HB3  | 2.14                     | 0.47              |
| 2:B:278:LEU:HD11 | 2:B:354:PHE:HB3   | 1.95                     | 0.47              |
| 2:B:961:TYR:CZ   | 2:B:965:MET:HE2   | 2.49                     | 0.47              |
| 1:A:512:MET:HG3  | 1:A:512:MET:O     | 2.15                     | 0.47              |
| 1:A:713:GLY:O    | 6:H:20:LYS:HE2    | 2.15                     | 0.47              |
| 1:A:1318:ARG:HB2 | 1:A:1526:GLN:HB3  | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1580:THR:HG22 | 1:A:1581:GLU:N    | 2.29                     | 0.47              |
| 2:B:1026:ILE:HG21 | 2:B:1031:VAL:HG12 | 1.96                     | 0.47              |
| 3:C:31:GLY:HA2    | 3:C:37:ASP:OD1    | 2.15                     | 0.47              |
| 3:C:299:LEU:HD23  | 3:C:299:LEU:H     | 1.79                     | 0.47              |
| 4:E:53:PRO:HB2    | 4:E:54:ARG:CZ     | 2.45                     | 0.47              |
| 9:K:62:ASN:O      | 9:K:65:VAL:HG22   | 2.15                     | 0.47              |
| 1:A:181:VAL:HG11  | 4:E:166:ARG:NH2   | 2.30                     | 0.47              |
| 1:A:558:ARG:HB3   | 1:A:559:PRO:HD3   | 1.96                     | 0.47              |
| 1:A:1518:ASP:CB   | 1:A:1522:SER:HA   | 2.44                     | 0.47              |
| 2:B:332:ILE:HG13  | 2:B:332:ILE:O     | 2.14                     | 0.47              |
| 2:B:337:LYS:HB2   | 2:B:337:LYS:HE2   | 1.66                     | 0.47              |
| 2:B:742:ILE:HD12  | 8:J:43:TYR:CE1    | 2.50                     | 0.47              |
| 3:C:240:THR:CG2   | 3:C:298:ARG:HB3   | 2.44                     | 0.47              |
| 6:H:105:SER:O     | 6:H:106:THR:HB    | 2.14                     | 0.47              |
| 7:I:55:VAL:HA     | 7:I:59:VAL:CG1    | 2.45                     | 0.47              |
| 1:A:258:PRO:HD2   | 1:A:391:TRP:CE3   | 2.50                     | 0.46              |
| 1:A:464:THR:HG22  | 1:A:464:THR:O     | 2.14                     | 0.46              |
| 1:A:1085:ARG:NH2  | 4:E:19:GLN:HG2    | 2.30                     | 0.46              |
| 1:A:1162:THR:HG21 | 4:E:199:THR:O     | 2.14                     | 0.46              |
| 1:A:1354:ILE:HD12 | 1:A:1540:MET:CE   | 2.45                     | 0.46              |
| 2:B:64:PHE:HE2    | 2:B:397:LYS:CB    | 2.25                     | 0.46              |
| 2:B:626:LEU:HD13  | 2:B:659:GLN:HB3   | 1.97                     | 0.46              |
| 3:C:147:THR:N     | 3:C:164:VAL:HG22  | 2.26                     | 0.46              |
| 1:A:140:ARG:NH1   | 1:A:144:ARG:HH12  | 2.09                     | 0.46              |
| 1:A:1565:ASN:HD22 | 1:A:1579:ASN:HD22 | 1.63                     | 0.46              |
| 1:A:1575:GLU:O    | 1:A:1576:LEU:HD22 | 2.15                     | 0.46              |
| 2:B:290:MET:HE2   | 2:B:294:CYS:HB2   | 1.97                     | 0.46              |
| 13:M:33:LEU:HD22  | 13:M:39:MET:CE    | 2.45                     | 0.46              |
| 1:A:89:ASN:HB3    | 1:A:299:LEU:HG    | 1.97                     | 0.46              |
| 1:A:417:ILE:HB    | 2:B:1126:MET:CE   | 2.46                     | 0.46              |
| 1:A:972:ARG:HD3   | 2:B:489:LEU:HD12  | 1.97                     | 0.46              |
| 2:B:791:SER:C     | 2:B:792:LEU:HD23  | 2.36                     | 0.46              |
| 3:C:15:VAL:HG12   | 3:C:298:ARG:NH2   | 2.30                     | 0.46              |
| 4:E:159:LEU:HD11  | 4:E:206:TYR:CD2   | 2.50                     | 0.46              |
| 5:F:71:LEU:HD12   | 5:F:71:LEU:O      | 2.15                     | 0.46              |
| 13:M:67:LEU:CG    | 13:M:69:TYR:CE1   | 2.98                     | 0.46              |
| 16:U:2:DT:H2"     | 16:U:3:DG:H5"     | 1.97                     | 0.46              |
| 1:A:595:ASN:HD22  | 2:B:1035:ILE:HD12 | 1.79                     | 0.46              |
| 1:A:1037:PHE:H    | 1:A:1038:PRO:HD2  | 1.78                     | 0.46              |
| 2:B:141:VAL:HB    | 2:B:167:GLY:HA3   | 1.97                     | 0.46              |
| 2:B:175:ILE:CG2   | 2:B:175:ILE:O     | 2.64                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:269:ILE:HD13  | 2:B:278:LEU:HD23  | 1.98                     | 0.46              |
| 2:B:910:VAL:O     | 8:J:9:THR:HG22    | 2.15                     | 0.46              |
| 2:B:926:ILE:O     | 2:B:926:ILE:HG22  | 2.15                     | 0.46              |
| 2:B:940:LEU:HD12  | 8:J:43:TYR:CB     | 2.41                     | 0.46              |
| 2:B:1037:PHE:CD2  | 2:B:1058:LEU:HD21 | 2.51                     | 0.46              |
| 2:B:1069:VAL:HG12 | 2:B:1076:LEU:HD13 | 1.97                     | 0.46              |
| 11:N:24:ALA:HB3   | 11:N:27:SER:HB3   | 1.98                     | 0.46              |
| 1:A:417:ILE:HB    | 2:B:1126:MET:HE3  | 1.97                     | 0.46              |
| 1:A:551:ASN:O     | 1:A:594:MET:HG3   | 2.15                     | 0.46              |
| 1:A:665:VAL:CG1   | 9:K:33:ALA:HB2    | 2.45                     | 0.46              |
| 1:A:869:VAL:HG21  | 1:A:918:GLN:NE2   | 2.20                     | 0.46              |
| 1:A:1106:GLU:O    | 1:A:1106:GLU:HG2  | 2.14                     | 0.46              |
| 2:B:66:PHE:CE1    | 2:B:75:PHE:CE2    | 3.02                     | 0.46              |
| 2:B:722:VAL:HG21  | 2:B:934:ALA:CB    | 2.44                     | 0.46              |
| 1:A:936:PRO:HG2   | 2:B:494:TRP:HB3   | 1.97                     | 0.46              |
| 2:B:386:LYS:O     | 2:B:390:GLU:HG3   | 2.16                     | 0.46              |
| 2:B:393:LEU:O     | 2:B:396:ILE:HG12  | 2.16                     | 0.46              |
| 2:B:403:LYS:HB3   | 2:B:418:ARG:NH2   | 2.26                     | 0.46              |
| 2:B:705:ASP:HA    | 2:B:853:LYS:HZ3   | 1.79                     | 0.46              |
| 3:C:138:LEU:HD21  | 3:C:190:ILE:HG21  | 1.98                     | 0.46              |
| 3:C:339:GLU:HG2   | 9:K:26:ALA:HB3    | 1.97                     | 0.46              |
| 13:M:81:CYS:SG    | 13:M:85:CYS:SG    | 3.05                     | 0.46              |
| 1:A:1669:LEU:HD23 | 1:A:1669:LEU:HA   | 1.81                     | 0.46              |
| 2:B:39:THR:HG21   | 2:B:166:MET:HG2   | 1.98                     | 0.46              |
| 2:B:632:GLU:HG2   | 2:B:633:LEU:N     | 2.31                     | 0.46              |
| 2:B:808:ASP:O     | 2:B:809:ASP:HB2   | 2.15                     | 0.46              |
| 2:B:821:TYR:HB2   | 2:B:844:LYS:HZ2   | 1.80                     | 0.46              |
| 6:H:35:PHE:HB3    | 6:H:37:MET:HG3    | 1.96                     | 0.46              |
| 1:A:221:SER:HA    | 1:A:395:GLN:HG2   | 1.98                     | 0.46              |
| 1:A:497:VAL:HG13  | 1:A:505:THR:CG2   | 2.45                     | 0.46              |
| 1:A:498:ILE:O     | 1:A:536:LYS:HA    | 2.16                     | 0.46              |
| 2:B:333:CYS:SG    | 2:B:345:MET:SD    | 3.13                     | 0.46              |
| 10:L:37:ARG:O     | 10:L:38:GLU:HB3   | 2.15                     | 0.46              |
| 13:M:28:PHE:CZ    | 13:M:33:LEU:HD11  | 2.50                     | 0.46              |
| 1:A:430:LYS:O     | 1:A:431:HIS:HB2   | 2.16                     | 0.46              |
| 1:A:1318:ARG:HD2  | 1:A:1524:TRP:CE3  | 2.48                     | 0.46              |
| 2:B:39:THR:CG2    | 2:B:166:MET:HG2   | 2.45                     | 0.46              |
| 2:B:269:ILE:HG22  | 2:B:273:GLU:HA    | 1.98                     | 0.46              |
| 2:B:471:CYS:SG    | 2:B:511:MET:HG2   | 2.56                     | 0.46              |
| 2:B:847:CYS:SG    | 2:B:871:MET:HG2   | 2.56                     | 0.46              |
| 3:C:245:VAL:HG21  | 3:C:253:LEU:HD22  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:I:29:LEU:N      | 7:I:41:CYS:HA     | 2.30                     | 0.46              |
| 9:K:90:LEU:HD12   | 9:K:95:PRO:HD3    | 1.98                     | 0.46              |
| 1:A:1348:LYS:HZ3  | 1:A:1509:HIS:HB3  | 1.81                     | 0.46              |
| 1:A:1533:LEU:H    | 1:A:1535:LYS:NZ   | 2.14                     | 0.46              |
| 2:B:700:LEU:HD11  | 2:B:706:ARG:CG    | 2.39                     | 0.46              |
| 2:B:707:SER:HB2   | 2:B:868:CYS:SG    | 2.56                     | 0.46              |
| 2:B:722:VAL:HG21  | 2:B:934:ALA:HB3   | 1.98                     | 0.46              |
| 3:C:61:LEU:HG     | 3:C:63:PHE:HD1    | 1.80                     | 0.46              |
| 5:F:55:PRO:O      | 5:F:123:LEU:HD12  | 2.16                     | 0.46              |
| 1:A:33:ILE:HD13   | 1:A:304:VAL:HG11  | 1.98                     | 0.45              |
| 1:A:214:VAL:HG21  | 1:A:216:ARG:NH2   | 2.30                     | 0.45              |
| 1:A:804:VAL:HG13  | 1:A:884:GLY:O     | 2.15                     | 0.45              |
| 1:A:1090:LEU:HD21 | 4:E:33:LEU:HD12   | 1.99                     | 0.45              |
| 1:A:1275:LEU:O    | 1:A:1278:VAL:HG12 | 2.15                     | 0.45              |
| 1:A:1288:VAL:HB   | 1:A:1331:LYS:HE3  | 1.98                     | 0.45              |
| 2:B:29:GLU:H      | 2:B:29:GLU:CD     | 2.20                     | 0.45              |
| 3:C:290:ASN:HD22  | 3:C:293:LEU:HB2   | 1.81                     | 0.45              |
| 3:C:337:LEU:HD12  | 9:K:104:MET:HE1   | 1.97                     | 0.45              |
| 4:E:125:TYR:O     | 4:E:127:LEU:HD12  | 2.16                     | 0.45              |
| 1:A:1000:VAL:HG12 | 1:A:1210:ALA:HA   | 1.96                     | 0.45              |
| 1:A:1343:GLU:HG3  | 1:A:1505:VAL:CG2  | 2.46                     | 0.45              |
| 2:B:905:THR:HG21  | 2:B:909:MET:HB2   | 1.98                     | 0.45              |
| 9:K:83:ARG:HH11   | 9:K:85:GLN:NE2    | 2.11                     | 0.45              |
| 11:N:38:PRO:O     | 13:M:94:LYS:NZ    | 2.47                     | 0.45              |
| 1:A:897:MET:SD    | 2:B:921:PRO:HG3   | 2.56                     | 0.45              |
| 2:B:183:ILE:HG13  | 2:B:472:VAL:HG12  | 1.98                     | 0.45              |
| 11:N:81:ARG:HB3   | 11:N:118:LEU:HG   | 1.98                     | 0.45              |
| 1:A:678:PRO:HB2   | 6:H:47:ILE:CG2    | 2.47                     | 0.45              |
| 2:B:167:GLY:O     | 2:B:169:TYR:CD2   | 2.68                     | 0.45              |
| 2:B:667:LEU:HD12  | 2:B:667:LEU:HA    | 1.86                     | 0.45              |
| 3:C:236:LEU:HD22  | 3:C:305:HIS:CD2   | 2.51                     | 0.45              |
| 3:C:261:VAL:HG21  | 3:C:281:ASP:HB2   | 1.97                     | 0.45              |
| 1:A:1511:PHE:HB3  | 1:A:1529:VAL:HG13 | 1.97                     | 0.45              |
| 2:B:336:LEU:CD2   | 2:B:561:VAL:HG22  | 2.46                     | 0.45              |
| 2:B:818:LYS:HG2   | 2:B:848:VAL:HG12  | 1.99                     | 0.45              |
| 1:A:972:ARG:HH11  | 2:B:489:LEU:HD12  | 1.82                     | 0.45              |
| 1:A:1184:LYS:HE3  | 1:A:1184:LYS:HB3  | 1.83                     | 0.45              |
| 1:A:1348:LYS:NZ   | 1:A:1509:HIS:HB3  | 2.32                     | 0.45              |
| 1:A:1512:ILE:HG22 | 1:A:1513:ASP:N    | 2.31                     | 0.45              |
| 2:B:149:ARG:O     | 2:B:150:ASN:HB2   | 2.17                     | 0.45              |
| 2:B:238:PHE:CE1   | 2:B:327:LEU:HD11  | 2.51                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:247:LEU:HD12 | 2:B:248:PRO:HD2  | 1.98                     | 0.45              |
| 4:E:11:TRP:HB2   | 4:E:40:PHE:CD2   | 2.52                     | 0.45              |
| 4:E:92:GLN:HA    | 4:E:95:GLN:CD    | 2.37                     | 0.45              |
| 5:F:122:GLU:O    | 5:F:122:GLU:HG3  | 2.15                     | 0.45              |
| 13:M:67:LEU:HD11 | 13:M:69:TYR:CE1  | 2.52                     | 0.45              |
| 1:A:716:TRP:HZ2  | 1:A:748:VAL:HG11 | 1.80                     | 0.45              |
| 2:B:75:PHE:CD2   | 2:B:75:PHE:N     | 2.82                     | 0.45              |
| 2:B:800:ASP:HB3  | 2:B:803:VAL:HG22 | 1.99                     | 0.45              |
| 3:C:193:VAL:HG11 | 3:C:314:GLY:HA3  | 1.99                     | 0.45              |
| 6:H:63:THR:HG22  | 6:H:71:ASP:OD1   | 2.17                     | 0.45              |
| 1:A:619:LEU:HD23 | 1:A:626:PRO:HA   | 1.99                     | 0.45              |
| 1:A:1128:ASP:CB  | 1:A:1133:ARG:HD3 | 2.46                     | 0.45              |
| 1:A:1531:LEU:CB  | 1:A:1535:LYS:HD3 | 2.47                     | 0.45              |
| 2:B:400:PHE:HA   | 2:B:418:ARG:NH1  | 2.30                     | 0.45              |
| 2:B:797:LYS:HE2  | 2:B:797:LYS:HB3  | 1.82                     | 0.45              |
| 3:C:236:LEU:HB2  | 3:C:305:HIS:HD2  | 1.82                     | 0.45              |
| 9:K:22:GLU:HG2   | 9:K:25:THR:CB    | 2.46                     | 0.45              |
| 1:A:138:LEU:HD11 | 1:A:165:THR:CG2  | 2.42                     | 0.45              |
| 1:A:387:LEU:HD12 | 1:A:390:ILE:HD11 | 1.97                     | 0.45              |
| 2:B:35:LEU:HD13  | 2:B:35:LEU:HA    | 1.86                     | 0.45              |
| 2:B:336:LEU:HD22 | 2:B:561:VAL:HG22 | 1.99                     | 0.45              |
| 2:B:810:ASP:OD2  | 10:L:17:TYR:OH   | 2.30                     | 0.45              |
| 13:M:16:ALA:HB3  | 13:M:19:GLY:HA2  | 1.98                     | 0.45              |
| 1:A:105:LEU:HD12 | 1:A:264:HIS:CE1  | 2.52                     | 0.45              |
| 1:A:651:GLU:HG3  | 9:K:60:MET:HE3   | 1.99                     | 0.45              |
| 1:A:1589:PHE:HA  | 1:A:1597:LEU:CD1 | 2.47                     | 0.45              |
| 2:B:98:VAL:O     | 2:B:110:TYR:HE1  | 2.00                     | 0.45              |
| 2:B:689:CYS:O    | 2:B:693:LYS:HD3  | 2.17                     | 0.45              |
| 2:B:698:PHE:HE2  | 2:B:701:LEU:HD23 | 1.80                     | 0.45              |
| 2:B:721:LEU:HD21 | 8:J:50:LEU:HD23  | 1.97                     | 0.45              |
| 2:B:792:LEU:CD1  | 2:B:865:LYS:HD2  | 2.41                     | 0.45              |
| 2:B:853:LYS:HE2  | 10:L:45:TYR:HE2  | 1.82                     | 0.45              |
| 4:E:13:ILE:CD1   | 4:E:132:GLN:HG3  | 2.47                     | 0.45              |
| 8:J:24:LEU:O     | 8:J:29:TYR:HB2   | 2.17                     | 0.45              |
| 2:B:92:ILE:CG2   | 2:B:93:CYS:H     | 2.24                     | 0.44              |
| 2:B:184:MET:HB3  | 2:B:185:PRO:HD2  | 1.98                     | 0.44              |
| 2:B:205:TYR:CD1  | 2:B:229:LEU:HD22 | 2.52                     | 0.44              |
| 2:B:284:GLN:O    | 2:B:288:ILE:HB   | 2.17                     | 0.44              |
| 3:C:241:LEU:HD21 | 3:C:253:LEU:HD21 | 1.99                     | 0.44              |
| 1:A:174:LEU:HG   | 1:A:174:LEU:O    | 2.17                     | 0.44              |
| 1:A:854:ASP:O    | 1:A:855:GLN:HB2  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:760:ASN:OD1  | 2:B:761:LYS:N     | 2.50                     | 0.44              |
| 4:E:168:ASN:HA   | 4:E:172:ARG:HH12  | 1.82                     | 0.44              |
| 1:A:715:ALA:HB2  | 1:A:899:GLN:NE2   | 2.33                     | 0.44              |
| 1:A:969:MET:CG   | 2:B:489:LEU:HD22  | 2.33                     | 0.44              |
| 2:B:5:SER:O      | 2:B:6:ARG:HB3     | 2.17                     | 0.44              |
| 2:B:758:ILE:HD12 | 2:B:895:ARG:HB2   | 1.95                     | 0.44              |
| 3:C:14:VAL:C     | 3:C:300:ALA:HB1   | 2.38                     | 0.44              |
| 5:F:53:THR:OG1   | 5:F:108:ARG:NH1   | 2.48                     | 0.44              |
| 13:M:39:MET:HG2  | 13:M:64:THR:HG22  | 1.99                     | 0.44              |
| 1:A:464:THR:O    | 1:A:464:THR:CG2   | 2.66                     | 0.44              |
| 1:A:518:VAL:HG22 | 1:A:518:VAL:O     | 2.17                     | 0.44              |
| 1:A:555:THR:HG23 | 2:B:1041:GLU:OE2  | 2.17                     | 0.44              |
| 1:A:833:LEU:HD22 | 1:A:833:LEU:HA    | 1.85                     | 0.44              |
| 1:A:1180:LYS:HD3 | 1:A:1180:LYS:HA   | 1.83                     | 0.44              |
| 1:A:1655:LYS:HB3 | 1:A:1655:LYS:HE3  | 1.69                     | 0.44              |
| 2:B:186:ARG:O    | 2:B:213:HIS:HB3   | 2.18                     | 0.44              |
| 2:B:197:LYS:HG2  | 2:B:197:LYS:O     | 2.18                     | 0.44              |
| 4:E:168:ASN:HA   | 4:E:172:ARG:HH22  | 1.83                     | 0.44              |
| 13:M:11:TRP:CZ2  | 13:M:101:VAL:HG11 | 2.53                     | 0.44              |
| 1:A:93:PHE:O     | 1:A:96:LEU:HB3    | 2.18                     | 0.44              |
| 1:A:422:GLU:HG2  | 1:A:1677:SER:HB3  | 1.99                     | 0.44              |
| 1:A:472:VAL:CG2  | 1:A:477:VAL:HG23  | 2.47                     | 0.44              |
| 1:A:598:PHE:O    | 1:A:600:GLN:HG2   | 2.18                     | 0.44              |
| 1:A:766:TYR:CD1  | 1:A:771:GLY:HA2   | 2.52                     | 0.44              |
| 1:A:987:TYR:CE2  | 1:A:1253:MET:HE1  | 2.52                     | 0.44              |
| 1:A:1628:VAL:O   | 1:A:1631:VAL:HG22 | 2.17                     | 0.44              |
| 2:B:526:TYR:O    | 2:B:527:THR:HG22  | 2.17                     | 0.44              |
| 4:E:87:ILE:HD11  | 4:E:110:MET:CE    | 2.48                     | 0.44              |
| 7:I:40:ARG:O     | 7:I:40:ARG:HG3    | 2.16                     | 0.44              |
| 13:M:69:TYR:HA   | 13:M:110:GLN:O    | 2.18                     | 0.44              |
| 1:A:268:LEU:HD23 | 1:A:268:LEU:O     | 2.16                     | 0.44              |
| 1:A:544:ASN:HA   | 1:A:566:ALA:O     | 2.17                     | 0.44              |
| 1:A:1113:ARG:O   | 1:A:1114:SER:HB2  | 2.17                     | 0.44              |
| 2:B:55:GLY:O     | 2:B:59:GLN:HG2    | 2.18                     | 0.44              |
| 6:H:56:PHE:HE1   | 6:H:58:LEU:HD12   | 1.83                     | 0.44              |
| 1:A:222:LYS:C    | 1:A:223:LEU:HD12  | 2.38                     | 0.44              |
| 1:A:716:TRP:CZ2  | 1:A:748:VAL:HG11  | 2.53                     | 0.44              |
| 1:A:801:ASP:HB3  | 1:A:887:ARG:HD2   | 2.00                     | 0.44              |
| 2:B:106:ARG:HG3  | 10:L:43:ILE:HD11  | 1.98                     | 0.44              |
| 2:B:239:ILE:HB   | 2:B:244:LEU:HD23  | 1.99                     | 0.44              |
| 2:B:525:VAL:HG21 | 2:B:590:PRO:HG3   | 2.00                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:647:PHE:CE1   | 2:B:663:PRO:HB3  | 2.53                     | 0.44              |
| 2:B:651:VAL:HG22  | 2:B:656:THR:HG21 | 1.99                     | 0.44              |
| 2:B:655:VAL:HG12  | 2:B:656:THR:N    | 2.32                     | 0.44              |
| 2:B:781:LEU:HD22  | 2:B:792:LEU:CB   | 2.37                     | 0.44              |
| 2:B:804:LEU:HG    | 2:B:805:GLN:OE1  | 2.18                     | 0.44              |
| 6:H:40:ILE:O      | 6:H:123:MET:HA   | 2.17                     | 0.44              |
| 1:A:812:ARG:HH11  | 1:A:914:CYS:C    | 2.21                     | 0.44              |
| 1:A:865:PHE:CZ    | 1:A:945:PRO:HA   | 2.53                     | 0.44              |
| 2:B:688:GLN:OE1   | 2:B:688:GLN:HA   | 2.18                     | 0.44              |
| 2:B:767:GLY:HA2   | 2:B:770:HIS:CE1  | 2.53                     | 0.44              |
| 2:B:828:TYR:CD1   | 2:B:828:TYR:N    | 2.86                     | 0.44              |
| 3:C:30:PRO:HG3    | 9:K:61:LYS:HA    | 1.99                     | 0.44              |
| 3:C:142:LEU:HD21  | 3:C:168:VAL:HG11 | 1.99                     | 0.44              |
| 7:I:14:GLN:CG     | 7:I:17:LEU:HD12  | 2.47                     | 0.44              |
| 1:A:1598:ARG:O    | 1:A:1599:ARG:HB2 | 2.17                     | 0.44              |
| 2:B:92:ILE:HG21   | 10:L:42:ARG:NH1  | 2.32                     | 0.44              |
| 2:B:1084:PRO:HD3  | 2:B:1094:ARG:NH2 | 2.33                     | 0.44              |
| 11:N:30:PHE:O     | 11:N:96:ALA:HB1  | 2.18                     | 0.44              |
| 11:N:84:SER:OG    | 11:N:115:LEU:CD2 | 2.66                     | 0.44              |
| 15:T:-5:DG:H2"    | 15:T:-4:DA:H8    | 1.82                     | 0.44              |
| 1:A:29:SER:HB3    | 1:A:80:HIS:HD2   | 1.81                     | 0.43              |
| 1:A:860:MET:HE2   | 1:A:864:LYS:CE   | 2.38                     | 0.43              |
| 1:A:1348:LYS:O    | 1:A:1352:GLU:HG3 | 2.18                     | 0.43              |
| 2:B:18:HIS:HE1    | 2:B:723:ARG:HH22 | 1.66                     | 0.43              |
| 2:B:109:THR:HA    | 2:B:171:ILE:O    | 2.18                     | 0.43              |
| 2:B:116:ALA:H     | 2:B:134:LEU:HD23 | 1.83                     | 0.43              |
| 2:B:162:GLU:C     | 2:B:164:GLU:N    | 2.72                     | 0.43              |
| 2:B:811:GLY:O     | 2:B:812:LEU:HD23 | 2.18                     | 0.43              |
| 4:E:122:ALA:O     | 4:E:124:LYS:N    | 2.50                     | 0.43              |
| 1:A:56:GLY:HA2    | 1:A:64:CYS:HB3   | 2.00                     | 0.43              |
| 1:A:64:CYS:SG     | 1:A:67:CYS:O     | 2.75                     | 0.43              |
| 1:A:100:LEU:HD21  | 1:A:265:LEU:CD2  | 2.48                     | 0.43              |
| 1:A:472:VAL:O     | 1:A:535:THR:HG21 | 2.18                     | 0.43              |
| 1:A:654:MET:C     | 1:A:656:LEU:H    | 2.22                     | 0.43              |
| 1:A:1357:LYS:HZ1  | 1:A:1538:PHE:HE1 | 1.66                     | 0.43              |
| 2:B:115:THR:HG22  | 2:B:133:PHE:HA   | 1.99                     | 0.43              |
| 2:B:156:LEU:HG    | 2:B:161:GLU:HB2  | 2.00                     | 0.43              |
| 2:B:743:VAL:HG21  | 2:B:997:VAL:CG2  | 2.47                     | 0.43              |
| 2:B:782:SER:HA    | 2:B:792:LEU:HD13 | 2.00                     | 0.43              |
| 2:B:1132:LEU:HD12 | 2:B:1132:LEU:O   | 2.18                     | 0.43              |
| 3:C:75:ALA:O      | 3:C:79:ILE:HG12  | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:I:30:PRO:O      | 7:I:31:GLY:C      | 2.57                     | 0.43              |
| 1:A:40:ASP:HB2    | 1:A:44:ASN:O      | 2.18                     | 0.43              |
| 1:A:186:GLU:HB2   | 1:A:1664:SER:HB2  | 2.00                     | 0.43              |
| 1:A:218:GLU:HG2   | 1:A:219:HIS:H     | 1.82                     | 0.43              |
| 1:A:976:VAL:O     | 1:A:980:VAL:HG13  | 2.18                     | 0.43              |
| 1:A:1300:GLN:HE22 | 7:I:48:ARG:HD3    | 1.83                     | 0.43              |
| 2:B:175:ILE:O     | 2:B:175:ILE:HG22  | 2.18                     | 0.43              |
| 2:B:403:LYS:CB    | 2:B:418:ARG:HH12  | 2.20                     | 0.43              |
| 3:C:149:ASN:OD1   | 3:C:161:GLU:HA    | 2.17                     | 0.43              |
| 6:H:92:MET:HE1    | 6:H:121:LEU:HD12  | 2.00                     | 0.43              |
| 6:H:118:TYR:OH    | 6:H:143:LEU:HB2   | 2.18                     | 0.43              |
| 11:N:39:ASP:HA    | 13:M:94:LYS:HE3   | 1.99                     | 0.43              |
| 1:A:433:MET:HB3   | 2:B:1039:GLU:HG2  | 1.98                     | 0.43              |
| 1:A:595:ASN:HB3   | 2:B:1035:ILE:HD12 | 2.00                     | 0.43              |
| 2:B:143:SER:O     | 2:B:144:LYS:HB2   | 2.18                     | 0.43              |
| 2:B:295:SER:HB3   | 7:I:34:ASP:OD2    | 2.19                     | 0.43              |
| 4:E:82:VAL:HG13   | 4:E:86:THR:HB     | 1.99                     | 0.43              |
| 9:K:65:VAL:HA     | 9:K:86:THR:HA     | 2.00                     | 0.43              |
| 13:M:33:LEU:HD13  | 13:M:39:MET:SD    | 2.59                     | 0.43              |
| 1:A:26:LYS:O      | 1:A:27:LYS:HB2    | 2.18                     | 0.43              |
| 1:A:553:GLN:HG2   | 15:T:3:DG:O4'     | 2.18                     | 0.43              |
| 1:A:745:LEU:HD21  | 6:H:95:LYS:HD3    | 2.00                     | 0.43              |
| 1:A:1531:LEU:HB3  | 1:A:1535:LYS:HD3  | 1.99                     | 0.43              |
| 2:B:63:PRO:HB3    | 2:B:76:THR:HG22   | 2.00                     | 0.43              |
| 2:B:240:TYR:HB2   | 2:B:331:CYS:SG    | 2.58                     | 0.43              |
| 4:E:43:GLN:O      | 4:E:44:SER:HB3    | 2.18                     | 0.43              |
| 4:E:67:ASP:CG     | 4:E:70:ASP:HB2    | 2.39                     | 0.43              |
| 4:E:87:ILE:HD11   | 4:E:110:MET:HE1   | 2.01                     | 0.43              |
| 6:H:32:SER:HB3    | 6:H:37:MET:H      | 1.83                     | 0.43              |
| 1:A:186:GLU:HG2   | 1:A:190:LYS:HE3   | 2.01                     | 0.43              |
| 1:A:718:LYS:HB3   | 1:A:718:LYS:HE2   | 1.82                     | 0.43              |
| 1:A:812:ARG:HD2   | 1:A:914:CYS:CA    | 2.46                     | 0.43              |
| 1:A:1095:LYS:O    | 1:A:1098:GLU:HB3  | 2.19                     | 0.43              |
| 2:B:625:ASN:O     | 2:B:629:GLY:N     | 2.48                     | 0.43              |
| 2:B:856:SER:CB    | 10:L:42:ARG:HB3   | 2.43                     | 0.43              |
| 3:C:56:MET:HE2    | 9:K:121:TYR:HD2   | 1.83                     | 0.43              |
| 4:E:56:THR:O      | 4:E:56:THR:HG22   | 2.18                     | 0.43              |
| 4:E:73:PHE:HB2    | 4:E:99:ILE:HD13   | 2.00                     | 0.43              |
| 4:E:143:GLU:HG3   | 4:E:144:LEU:HG    | 2.00                     | 0.43              |
| 4:E:179:VAL:O     | 4:E:179:VAL:HG12  | 2.18                     | 0.43              |
| 1:A:459:PRO:O     | 1:A:461:VAL:N     | 2.52                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:472:VAL:HG12  | 1:A:536:LYS:O     | 2.19                     | 0.43              |
| 1:A:754:TYR:CE1   | 1:A:781:LEU:HD22  | 2.54                     | 0.43              |
| 1:A:846:TRP:NE1   | 1:A:858:PHE:HE1   | 2.13                     | 0.43              |
| 1:A:866:LYS:O     | 1:A:869:VAL:HG22  | 2.19                     | 0.43              |
| 1:A:1006:THR:CG2  | 1:A:1008:ARG:HE   | 2.29                     | 0.43              |
| 1:A:1114:SER:HB3  | 1:A:1117:THR:H    | 1.84                     | 0.43              |
| 1:A:1583:ILE:CD1  | 1:A:1604:ASP:HB2  | 2.48                     | 0.43              |
| 1:A:1631:VAL:HG23 | 1:A:1632:TYR:CE2  | 2.53                     | 0.43              |
| 2:B:69:LYS:HE2    | 2:B:69:LYS:HB3    | 1.57                     | 0.43              |
| 3:C:100:ILE:HG13  | 8:J:60:LEU:HD23   | 2.00                     | 0.43              |
| 16:U:3:DG:H2'     | 16:U:4:DT:C6      | 2.53                     | 0.43              |
| 1:A:205:CYS:HB3   | 1:A:208:CYS:O     | 2.19                     | 0.43              |
| 1:A:811:LYS:O     | 1:A:815:ILE:HG13  | 2.18                     | 0.43              |
| 1:A:1531:LEU:O    | 1:A:1535:LYS:HD3  | 2.19                     | 0.43              |
| 2:B:18:HIS:O      | 2:B:21:ASP:HB2    | 2.19                     | 0.43              |
| 2:B:32:LYS:O      | 2:B:33:ALA:HB3    | 2.19                     | 0.43              |
| 2:B:388:LYS:HE3   | 2:B:429:PRO:HB3   | 2.01                     | 0.43              |
| 2:B:432:TYR:HE1   | 15:T:10:DA:H5''   | 1.82                     | 0.43              |
| 9:K:89:THR:HG23   | 9:K:90:LEU:H      | 1.81                     | 0.43              |
| 1:A:30:VAL:CG1    | 1:A:66:THR:HG21   | 2.49                     | 0.43              |
| 1:A:454:ASN:HA    | 1:A:614:THR:HG21  | 2.00                     | 0.43              |
| 1:A:513:THR:HG23  | 1:A:514:GLN:N     | 2.34                     | 0.43              |
| 1:A:896:MET:HG3   | 1:A:896:MET:O     | 2.19                     | 0.43              |
| 1:A:1134:LYS:HE2  | 1:A:1134:LYS:CA   | 2.49                     | 0.43              |
| 1:A:1300:GLN:NE2  | 7:I:48:ARG:HD3    | 2.34                     | 0.43              |
| 1:A:1566:GLU:O    | 1:A:1576:LEU:HD22 | 2.19                     | 0.43              |
| 1:A:1639:ARG:HE   | 4:E:199:THR:HG21  | 1.83                     | 0.43              |
| 2:B:172:ILE:O     | 2:B:173:ASN:HB2   | 2.17                     | 0.43              |
| 2:B:248:PRO:HB2   | 2:B:251:PHE:HD2   | 1.82                     | 0.43              |
| 3:C:246:GLU:HG2   | 3:C:272:VAL:HA    | 2.01                     | 0.43              |
| 1:A:131:ALA:HB2   | 1:A:172:ASN:HD22  | 1.83                     | 0.43              |
| 1:A:404:SER:CB    | 1:A:415:PRO:HA    | 2.42                     | 0.43              |
| 1:A:642:THR:HB    | 1:A:748:VAL:O     | 2.19                     | 0.43              |
| 1:A:833:LEU:HD13  | 1:A:834:PRO:HD2   | 2.00                     | 0.43              |
| 1:A:980:VAL:HG11  | 2:B:484:THR:HG21  | 2.01                     | 0.43              |
| 1:A:1515:TYR:O    | 1:A:1526:GLN:NE2  | 2.52                     | 0.43              |
| 1:A:1523:LEU:HD12 | 1:A:1524:TRP:HB2  | 2.01                     | 0.43              |
| 2:B:258:SER:HB3   | 2:B:297:GLN:OE1   | 2.19                     | 0.43              |
| 2:B:430:PHE:O     | 2:B:434:PHE:HD1   | 2.02                     | 0.43              |
| 2:B:804:LEU:N     | 2:B:804:LEU:HD23  | 2.34                     | 0.43              |
| 3:C:102:GLN:O     | 3:C:106:LEU:HB2   | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:337:LEU:HD21  | 9:K:100:LEU:CB    | 2.49                     | 0.43              |
| 11:N:29:ARG:C     | 11:N:31:SER:H     | 2.22                     | 0.43              |
| 1:A:217:LYS:HD2   | 1:A:218:GLU:O     | 2.19                     | 0.42              |
| 1:A:431:HIS:O     | 2:B:1115:VAL:HG11 | 2.19                     | 0.42              |
| 1:A:602:GLU:O     | 1:A:602:GLU:HG3   | 2.19                     | 0.42              |
| 1:A:680:PRO:HG2   | 3:C:31:GLY:O      | 2.18                     | 0.42              |
| 1:A:1129:GLU:OE1  | 1:A:1132:ARG:CB   | 2.67                     | 0.42              |
| 1:A:1133:ARG:O    | 1:A:1133:ARG:CG   | 2.66                     | 0.42              |
| 1:A:1251:ILE:O    | 1:A:1654:TYR:OH   | 2.30                     | 0.42              |
| 1:A:1605:ILE:HG21 | 1:A:1621:ILE:HG13 | 1.98                     | 0.42              |
| 2:B:214:CYS:O     | 2:B:221:ALA:HA    | 2.19                     | 0.42              |
| 2:B:370:VAL:HG13  | 2:B:637:MET:HA    | 2.01                     | 0.42              |
| 2:B:519:GLU:HG3   | 2:B:620:VAL:HG23  | 2.01                     | 0.42              |
| 2:B:704:GLN:HG3   | 2:B:704:GLN:O     | 2.18                     | 0.42              |
| 2:B:908:GLY:HA2   | 3:C:232:SER:OG    | 2.19                     | 0.42              |
| 11:N:56:PHE:HZ    | 11:N:80:TYR:HB2   | 1.83                     | 0.42              |
| 1:A:1062:PRO:HB3  | 1:A:1156:PHE:HD2  | 1.83                     | 0.42              |
| 1:A:1111:ASN:ND2  | 4:E:61:LEU:HD23   | 2.34                     | 0.42              |
| 1:A:1615:GLU:OE2  | 4:E:207:ARG:NE    | 2.46                     | 0.42              |
| 1:A:1670:GLN:C    | 1:A:1672:MET:H    | 2.22                     | 0.42              |
| 2:B:863:LYS:O     | 2:B:865:LYS:HG2   | 2.19                     | 0.42              |
| 2:B:920:PHE:N     | 2:B:921:PRO:CD    | 2.83                     | 0.42              |
| 2:B:1003:ARG:O    | 2:B:1003:ARG:CD   | 2.64                     | 0.42              |
| 3:C:30:PRO:HB3    | 3:C:38:ASP:O      | 2.19                     | 0.42              |
| 6:H:107:GLU:HG3   | 6:H:108:ALA:N     | 2.34                     | 0.42              |
| 11:N:61:VAL:HG21  | 13:M:11:TRP:HE3   | 1.84                     | 0.42              |
| 11:N:142:PRO:CG   | 11:N:145:LEU:CD2  | 2.43                     | 0.42              |
| 11:N:146:ARG:NH1  | 11:N:148:ARG:NH2  | 2.63                     | 0.42              |
| 1:A:1009:ASP:OD1  | 1:A:1010:SER:N    | 2.47                     | 0.42              |
| 1:A:1334:ARG:HG3  | 1:A:1335:PRO:CD   | 2.40                     | 0.42              |
| 2:B:116:ALA:N     | 2:B:134:LEU:HD23  | 2.34                     | 0.42              |
| 2:B:720:PRO:O     | 2:B:723:ARG:HD3   | 2.19                     | 0.42              |
| 7:I:7:ALA:HA      | 7:I:15:SER:OG     | 2.19                     | 0.42              |
| 1:A:127:LEU:HD21  | 1:A:135:VAL:HG21  | 1.98                     | 0.42              |
| 1:A:408:LYS:HD3   | 1:A:408:LYS:H     | 1.85                     | 0.42              |
| 1:A:427:LEU:HG    | 1:A:427:LEU:O     | 2.19                     | 0.42              |
| 1:A:703:LEU:HD23  | 1:A:703:LEU:H     | 1.84                     | 0.42              |
| 1:A:961:PRO:N     | 1:A:962:PRO:HD2   | 2.33                     | 0.42              |
| 1:A:972:ARG:NH2   | 2:B:509:GLY:HA2   | 2.35                     | 0.42              |
| 1:A:1715:LEU:HD23 | 1:A:1715:LEU:HA   | 1.85                     | 0.42              |
| 2:B:73:ILE:HG22   | 2:B:75:PHE:CZ     | 2.51                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:269:ILE:HG22  | 2:B:269:ILE:O     | 2.19                     | 0.42              |
| 2:B:796:ILE:HD11  | 2:B:807:LEU:CB    | 2.41                     | 0.42              |
| 1:A:12:LEU:CD2    | 2:B:1132:LEU:HD13 | 2.49                     | 0.42              |
| 1:A:225:ILE:CG2   | 1:A:256:LEU:HD11  | 2.49                     | 0.42              |
| 1:A:636:VAL:HG11  | 1:A:795:PHE:CE1   | 2.54                     | 0.42              |
| 1:A:659:ARG:HD3   | 1:A:787:ALA:HB1   | 2.01                     | 0.42              |
| 2:B:210:VAL:HG21  | 2:B:349:MET:HB3   | 2.01                     | 0.42              |
| 2:B:576:ASP:OD1   | 2:B:576:ASP:C     | 2.57                     | 0.42              |
| 2:B:790:SER:C     | 2:B:792:LEU:H     | 2.22                     | 0.42              |
| 2:B:997:VAL:CG2   | 2:B:999:TYR:CE2   | 3.02                     | 0.42              |
| 3:C:40:TRP:HZ2    | 9:K:106:VAL:CG2   | 2.33                     | 0.42              |
| 1:A:463:ALA:CB    | 1:A:568:ILE:HD12  | 2.49                     | 0.42              |
| 1:A:1045:GLU:H    | 1:A:1045:GLU:HG2  | 1.43                     | 0.42              |
| 1:A:1092:TYR:CZ   | 1:A:1095:LYS:HD2  | 2.55                     | 0.42              |
| 1:A:1243:LEU:O    | 1:A:1246:PRO:HG2  | 2.19                     | 0.42              |
| 1:A:1618:LEU:HD11 | 1:A:1649:CYS:CB   | 2.49                     | 0.42              |
| 2:B:194:ILE:HD12  | 2:B:363:GLU:HB2   | 2.01                     | 0.42              |
| 2:B:691:MET:HE1   | 2:B:884:ALA:HB1   | 2.02                     | 0.42              |
| 2:B:746:ILE:CG2   | 2:B:914:LEU:HD22  | 2.50                     | 0.42              |
| 1:A:78:LEU:HD12   | 1:A:306:PRO:HD3   | 2.01                     | 0.42              |
| 1:A:121:LEU:HD23  | 1:A:125:ARG:HG3   | 2.01                     | 0.42              |
| 1:A:711:ILE:HG13  | 1:A:750:ASP:OD2   | 2.19                     | 0.42              |
| 1:A:1037:PHE:N    | 1:A:1038:PRO:CD   | 2.82                     | 0.42              |
| 1:A:1086:ARG:HB2  | 1:A:1086:ARG:NH1  | 2.35                     | 0.42              |
| 1:A:1268:VAL:O    | 1:A:1268:VAL:HG12 | 2.20                     | 0.42              |
| 1:A:1535:LYS:HD2  | 1:A:1535:LYS:N    | 2.34                     | 0.42              |
| 2:B:346:LEU:HD23  | 2:B:346:LEU:HA    | 1.93                     | 0.42              |
| 2:B:489:LEU:O     | 2:B:489:LEU:HD23  | 2.20                     | 0.42              |
| 2:B:1027:GLY:H    | 2:B:1033:GLY:HA2  | 1.83                     | 0.42              |
| 3:C:50:ARG:HG3    | 3:C:66:VAL:HB     | 2.02                     | 0.42              |
| 3:C:86:THR:HA     | 3:C:119:PRO:CG    | 2.49                     | 0.42              |
| 3:C:138:LEU:HD12  | 3:C:138:LEU:HA    | 1.92                     | 0.42              |
| 5:F:100:ARG:HE    | 5:F:100:ARG:HB3   | 1.72                     | 0.42              |
| 7:I:13:PHE:CD1    | 7:I:20:CYS:HB3    | 2.55                     | 0.42              |
| 1:A:326:VAL:HG11  | 1:A:414:TYR:CE1   | 2.55                     | 0.42              |
| 1:A:330:ALA:HB1   | 1:A:397:HIS:ND1   | 2.35                     | 0.42              |
| 1:A:705:LEU:CD1   | 1:A:761:LEU:HA    | 2.49                     | 0.42              |
| 1:A:1016:GLN:OE1  | 1:A:1643:LEU:HD13 | 2.19                     | 0.42              |
| 1:A:1559:ILE:HG23 | 1:A:1580:THR:HG23 | 2.01                     | 0.42              |
| 1:A:1704:LYS:HE2  | 1:A:1704:LYS:HB3  | 1.74                     | 0.42              |
| 2:B:162:GLU:HB2   | 2:B:165:GLU:HB3   | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:844:LYS:HA    | 2:B:844:LYS:HD3   | 1.94                     | 0.42              |
| 3:C:236:LEU:HB2   | 3:C:305:HIS:CD2   | 2.55                     | 0.42              |
| 4:E:169:GLN:O     | 4:E:169:GLN:CG    | 2.67                     | 0.42              |
| 9:K:45:HIS:O      | 9:K:46:GLU:HB2    | 2.19                     | 0.42              |
| 1:A:860:MET:HE2   | 1:A:864:LYS:HG3   | 2.01                     | 0.42              |
| 1:A:939:GLU:HG2   | 1:A:940:PRO:N     | 2.34                     | 0.42              |
| 1:A:1104:LYS:HD2  | 1:A:1104:LYS:O    | 2.20                     | 0.42              |
| 1:A:1280:SER:O    | 1:A:1284:GLN:HB2  | 2.19                     | 0.42              |
| 2:B:60:ALA:O      | 2:B:61:ILE:C      | 2.58                     | 0.42              |
| 2:B:179:ILE:HD11  | 2:B:434:PHE:CE2   | 2.55                     | 0.42              |
| 2:B:668:SER:O     | 2:B:672:ASN:ND2   | 2.53                     | 0.42              |
| 2:B:1097:ASN:OD1  | 2:B:1104:SER:HB2  | 2.20                     | 0.42              |
| 3:C:135:ILE:H     | 3:C:135:ILE:HG12  | 1.48                     | 0.42              |
| 3:C:336:PHE:CZ    | 9:K:44:LEU:HB3    | 2.55                     | 0.42              |
| 4:E:103:LEU:HD21  | 4:E:130:PHE:CD2   | 2.55                     | 0.42              |
| 4:E:110:MET:SD    | 4:E:118:LEU:CD1   | 3.06                     | 0.42              |
| 5:F:110:LEU:HB3   | 5:F:111:PRO:HD2   | 2.01                     | 0.42              |
| 1:A:1268:VAL:HG23 | 1:A:1576:LEU:O    | 2.19                     | 0.42              |
| 1:A:1716:LYS:HD3  | 1:A:1716:LYS:HA   | 1.87                     | 0.42              |
| 2:B:167:GLY:O     | 2:B:169:TYR:HD2   | 2.02                     | 0.42              |
| 2:B:521:VAL:O     | 2:B:616:PRO:O     | 2.38                     | 0.42              |
| 2:B:1053:LEU:HD23 | 2:B:1053:LEU:HA   | 1.91                     | 0.42              |
| 3:C:240:THR:HG23  | 3:C:240:THR:O     | 2.20                     | 0.42              |
| 3:C:312:SER:HB3   | 3:C:321:LEU:HD11  | 2.01                     | 0.42              |
| 7:I:43:PHE:HE1    | 7:I:46:ASN:HA     | 1.84                     | 0.42              |
| 1:A:302:LEU:HD23  | 1:A:302:LEU:HA    | 1.82                     | 0.41              |
| 1:A:613:CYS:SG    | 1:A:614:THR:N     | 2.93                     | 0.41              |
| 1:A:889:PHE:O     | 1:A:890:PRO:C     | 2.56                     | 0.41              |
| 1:A:1266:VAL:HG12 | 1:A:1596:ASP:O    | 2.20                     | 0.41              |
| 2:B:75:PHE:CD1    | 2:B:120:TRP:CB    | 3.03                     | 0.41              |
| 2:B:171:ILE:CG2   | 2:B:174:GLY:HA2   | 2.47                     | 0.41              |
| 2:B:792:LEU:HD12  | 2:B:865:LYS:CD    | 2.40                     | 0.41              |
| 4:E:85:LYS:HE2    | 4:E:85:LYS:HB3    | 1.87                     | 0.41              |
| 6:H:86:ASP:C      | 6:H:88:PHE:H      | 2.23                     | 0.41              |
| 1:A:754:TYR:HE1   | 1:A:781:LEU:HD22  | 1.85                     | 0.41              |
| 1:A:896:MET:O     | 1:A:896:MET:CG    | 2.67                     | 0.41              |
| 1:A:1568:THR:HG21 | 1:A:1577:VAL:HG11 | 2.01                     | 0.41              |
| 4:E:6:GLU:O       | 4:E:10:LEU:HD13   | 2.19                     | 0.41              |
| 4:E:73:PHE:HD2    | 4:E:75:PHE:CZ     | 2.38                     | 0.41              |
| 1:A:543:LYS:O     | 1:A:543:LYS:CG    | 2.68                     | 0.41              |
| 1:A:1137:LYS:HD2  | 1:A:1137:LYS:HA   | 1.89                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1162:THR:O    | 1:A:1166:LYS:HG3  | 2.20                     | 0.41              |
| 1:A:1570:ASN:OD1  | 1:A:1571:LYS:N    | 2.53                     | 0.41              |
| 1:A:1672:MET:O    | 1:A:1677:SER:HB2  | 2.19                     | 0.41              |
| 2:B:804:LEU:HD23  | 2:B:804:LEU:H     | 1.85                     | 0.41              |
| 2:B:961:TYR:CE1   | 2:B:965:MET:HE2   | 2.55                     | 0.41              |
| 6:H:26:SER:HB3    | 6:H:45:ILE:HG21   | 2.02                     | 0.41              |
| 14:R:-7:G:H2'     | 14:R:-6:C:C6      | 2.55                     | 0.41              |
| 1:A:912:ILE:CG1   | 2:B:924:MET:HG2   | 2.50                     | 0.41              |
| 1:A:992:ILE:HD11  | 1:A:1252:LEU:HD13 | 2.01                     | 0.41              |
| 1:A:1090:LEU:CD2  | 4:E:30:GLN:HG2    | 2.34                     | 0.41              |
| 1:A:1247:ARG:HG2  | 1:A:1628:VAL:CG2  | 2.49                     | 0.41              |
| 1:A:1324:HIS:HD2  | 1:A:1328:GLN:HG3  | 1.84                     | 0.41              |
| 1:A:1504:ALA:O    | 1:A:1508:ILE:HG13 | 2.21                     | 0.41              |
| 6:H:39:LEU:HD12   | 6:H:125:LEU:HD13  | 2.00                     | 0.41              |
| 9:K:60:MET:SD     | 9:K:68:CYS:HB3    | 2.60                     | 0.41              |
| 13:M:33:LEU:HD22  | 13:M:39:MET:HE3   | 2.02                     | 0.41              |
| 13:M:73:ASN:ND2   | 13:M:105:GLU:OE1  | 2.50                     | 0.41              |
| 1:A:33:ILE:HD11   | 1:A:81:ILE:CG1    | 2.51                     | 0.41              |
| 1:A:433:MET:CB    | 2:B:1039:GLU:HG2  | 2.51                     | 0.41              |
| 1:A:661:LEU:HG    | 1:A:691:LEU:CD1   | 2.51                     | 0.41              |
| 1:A:866:LYS:HA    | 1:A:869:VAL:CG2   | 2.49                     | 0.41              |
| 2:B:185:PRO:O     | 2:B:186:ARG:HB2   | 2.21                     | 0.41              |
| 2:B:804:LEU:HG    | 2:B:805:GLN:N     | 2.36                     | 0.41              |
| 3:C:230:THR:HG23  | 8:J:10:CYS:HB2    | 2.01                     | 0.41              |
| 3:C:263:GLU:CB    | 3:C:276:ALA:HB2   | 2.50                     | 0.41              |
| 3:C:312:SER:HB3   | 3:C:321:LEU:HD12  | 2.02                     | 0.41              |
| 8:J:17:LYS:HE3    | 8:J:38:LEU:O      | 2.20                     | 0.41              |
| 13:M:81:CYS:O     | 13:M:85:CYS:SG    | 2.69                     | 0.41              |
| 1:A:215:VAL:HG22  | 1:A:225:ILE:CG2   | 2.50                     | 0.41              |
| 1:A:327:ASN:HB3   | 1:A:401:VAL:HG22  | 2.02                     | 0.41              |
| 1:A:737:VAL:HA    | 1:A:746:CYS:O     | 2.20                     | 0.41              |
| 1:A:811:LYS:HA    | 1:A:814:ARG:HG2   | 2.03                     | 0.41              |
| 1:A:1136:GLN:HE21 | 1:A:1136:GLN:HB3  | 1.63                     | 0.41              |
| 1:A:1324:HIS:CD2  | 1:A:1328:GLN:HG3  | 2.56                     | 0.41              |
| 1:A:1518:ASP:CG   | 1:A:1524:TRP:H    | 2.23                     | 0.41              |
| 1:A:1580:THR:CG2  | 1:A:1581:GLU:N    | 2.84                     | 0.41              |
| 2:B:35:LEU:HD13   | 2:B:730:TYR:HD2   | 1.85                     | 0.41              |
| 2:B:86:THR:HG22   | 2:B:87:VAL:N      | 2.35                     | 0.41              |
| 2:B:104:ARG:NH2   | 2:B:169:TYR:OH    | 2.52                     | 0.41              |
| 2:B:786:LYS:O     | 2:B:788:GLY:N     | 2.52                     | 0.41              |
| 1:A:674:SER:HB2   | 6:H:118:TYR:O     | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:850:HIS:HD2   | 1:A:941:TYR:OH    | 2.04                     | 0.41              |
| 1:A:1268:VAL:HG13 | 1:A:1595:LEU:HD23 | 2.01                     | 0.41              |
| 2:B:247:LEU:HD11  | 2:B:304:LEU:HD21  | 2.03                     | 0.41              |
| 2:B:396:ILE:HA    | 2:B:422:MET:CB    | 2.51                     | 0.41              |
| 2:B:566:VAL:HG23  | 2:B:574:ILE:HD12  | 2.02                     | 0.41              |
| 2:B:1066:VAL:O    | 2:B:1066:VAL:CG1  | 2.67                     | 0.41              |
| 13:M:67:LEU:CD1   | 13:M:68:SER:O     | 2.64                     | 0.41              |
| 1:A:95:LYS:HA     | 1:A:95:LYS:HD3    | 1.74                     | 0.41              |
| 1:A:445:ILE:HD11  | 1:A:587:ALA:HB1   | 2.03                     | 0.41              |
| 1:A:1078:LYS:HB2  | 1:A:1078:LYS:HE3  | 1.82                     | 0.41              |
| 1:A:1090:LEU:HD12 | 4:E:22:HIS:NE2    | 2.36                     | 0.41              |
| 2:B:416:LEU:HD12  | 2:B:419:ILE:HD11  | 2.02                     | 0.41              |
| 2:B:700:LEU:HA    | 2:B:735:TYR:HE1   | 1.85                     | 0.41              |
| 2:B:821:TYR:HD2   | 2:B:844:LYS:HZ2   | 1.64                     | 0.41              |
| 2:B:853:LYS:HG2   | 10:L:45:TYR:CE2   | 2.56                     | 0.41              |
| 2:B:1065:SER:HB2  | 2:B:1117:ARG:NH2  | 2.36                     | 0.41              |
| 2:B:1069:VAL:HG21 | 2:B:1134:VAL:CG2  | 2.50                     | 0.41              |
| 3:C:218:ILE:HD12  | 3:C:220:LYS:HB3   | 2.03                     | 0.41              |
| 3:C:245:VAL:O     | 3:C:246:GLU:HG3   | 2.21                     | 0.41              |
| 1:A:26:LYS:HE3    | 1:A:301:PHE:CE2   | 2.55                     | 0.41              |
| 1:A:61:LYS:HE3    | 1:A:61:LYS:HB2    | 1.86                     | 0.41              |
| 1:A:85:LEU:HD22   | 1:A:391:TRP:NE1   | 2.33                     | 0.41              |
| 1:A:441:ALA:HB2   | 2:B:1012:VAL:HG13 | 2.03                     | 0.41              |
| 1:A:468:TYR:HB2   | 1:A:598:PHE:CE2   | 2.56                     | 0.41              |
| 1:A:579:TYR:CE1   | 2:B:753:MET:HB2   | 2.56                     | 0.41              |
| 1:A:644:ARG:HE    | 1:A:644:ARG:HB2   | 1.70                     | 0.41              |
| 1:A:705:LEU:HD23  | 1:A:706:SER:N     | 2.36                     | 0.41              |
| 1:A:981:LYS:HE3   | 1:A:981:LYS:HB3   | 1.90                     | 0.41              |
| 1:A:1020:GLY:O    | 1:A:1021:GLU:HB2  | 2.20                     | 0.41              |
| 1:A:1300:GLN:O    | 1:A:1315:TYR:HA   | 2.20                     | 0.41              |
| 1:A:1602:SER:HB3  | 1:A:1608:ILE:HD11 | 2.02                     | 0.41              |
| 2:B:215:VAL:HA    | 2:B:220:SER:O     | 2.20                     | 0.41              |
| 2:B:364:ASP:OD1   | 2:B:606:LEU:HD22  | 2.21                     | 0.41              |
| 2:B:408:SER:HA    | 2:B:411:MET:CB    | 2.38                     | 0.41              |
| 2:B:820:GLN:O     | 2:B:823:ASP:HB2   | 2.21                     | 0.41              |
| 2:B:1026:ILE:HG21 | 2:B:1031:VAL:HG11 | 2.02                     | 0.41              |
| 3:C:89:VAL:HG22   | 3:C:214:CYS:SG    | 2.61                     | 0.41              |
| 3:C:186:PRO:CG    | 3:C:189:THR:OG1   | 2.63                     | 0.41              |
| 4:E:17:ILE:HG21   | 4:E:74:VAL:HG11   | 2.03                     | 0.41              |
| 4:E:159:LEU:CD2   | 4:E:160:LEU:HD23  | 2.45                     | 0.41              |
| 6:H:14:ASP:HB3    | 6:H:17:PRO:HG3    | 2.02                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:H:80:ASP:O      | 6:H:82:PRO:HD3   | 2.21                     | 0.41              |
| 9:K:93:VAL:O      | 9:K:93:VAL:HG12  | 2.21                     | 0.41              |
| 11:N:61:VAL:N     | 13:M:9:ALA:O     | 2.54                     | 0.41              |
| 11:N:70:LYS:HE2   | 11:N:79:ARG:NH1  | 2.36                     | 0.41              |
| 13:M:67:LEU:HD12  | 13:M:68:SER:N    | 2.36                     | 0.41              |
| 13:M:68:SER:HB2   | 13:M:112:LEU:HB2 | 2.02                     | 0.41              |
| 1:A:826:ALA:HB2   | 1:A:868:GLU:HG3  | 2.02                     | 0.41              |
| 1:A:1267:PRO:HG2  | 1:A:1596:ASP:HB3 | 2.03                     | 0.41              |
| 1:A:1583:ILE:HG23 | 1:A:1583:ILE:O   | 2.21                     | 0.41              |
| 2:B:82:ILE:HD13   | 2:B:137:VAL:HG21 | 2.02                     | 0.41              |
| 2:B:496:PHE:C     | 2:B:497:LEU:HD12 | 2.41                     | 0.41              |
| 2:B:1019:ASP:O    | 2:B:1023:ASN:N   | 2.50                     | 0.41              |
| 3:C:29:PHE:CE1    | 9:K:57:TYR:HE1   | 2.39                     | 0.41              |
| 3:C:157:SER:O     | 3:C:161:GLU:HG3  | 2.21                     | 0.41              |
| 6:H:125:LEU:HD12  | 6:H:125:LEU:HA   | 1.90                     | 0.41              |
| 9:K:22:GLU:CG     | 9:K:25:THR:H     | 2.25                     | 0.41              |
| 10:L:15:MET:HE3   | 10:L:15:MET:HA   | 2.03                     | 0.41              |
| 1:A:293:ASN:O     | 1:A:296:VAL:HG23 | 2.22                     | 0.40              |
| 1:A:498:ILE:O     | 1:A:536:LYS:HG3  | 2.21                     | 0.40              |
| 1:A:1289:CYS:SG   | 1:A:1549:HIS:O   | 2.80                     | 0.40              |
| 1:A:1639:ARG:HE   | 4:E:199:THR:CG2  | 2.34                     | 0.40              |
| 2:B:267:GLU:HA    | 2:B:270:LYS:HD3  | 2.02                     | 0.40              |
| 2:B:399:ALA:HB2   | 2:B:422:MET:CE   | 2.51                     | 0.40              |
| 2:B:1112:VAL:HG21 | 2:B:1116:PHE:CD2 | 2.56                     | 0.40              |
| 3:C:337:LEU:CD1   | 9:K:104:MET:HE3  | 2.49                     | 0.40              |
| 7:I:29:LEU:H      | 7:I:41:CYS:HA    | 1.86                     | 0.40              |
| 9:K:90:LEU:H      | 9:K:90:LEU:CD2   | 2.26                     | 0.40              |
| 1:A:102:GLY:O     | 1:A:103:SER:OG   | 2.31                     | 0.40              |
| 1:A:1106:GLU:O    | 1:A:1107:SER:OG  | 2.29                     | 0.40              |
| 2:B:146:CYS:O     | 2:B:149:ARG:NH1  | 2.47                     | 0.40              |
| 2:B:333:CYS:SG    | 2:B:333:CYS:O    | 2.79                     | 0.40              |
| 2:B:399:ALA:HB2   | 2:B:422:MET:SD   | 2.61                     | 0.40              |
| 2:B:543:ASP:HB2   | 13:M:81:CYS:HB2  | 2.03                     | 0.40              |
| 2:B:691:MET:HE3   | 2:B:884:ALA:HB1  | 2.02                     | 0.40              |
| 2:B:989:GLU:HG2   | 3:C:21:VAL:HG12  | 2.03                     | 0.40              |
| 2:B:1026:ILE:HD12 | 2:B:1026:ILE:HA  | 1.97                     | 0.40              |
| 3:C:40:TRP:HB2    | 9:K:61:LYS:HB3   | 2.02                     | 0.40              |
| 4:E:10:LEU:HD21   | 4:E:58:LEU:HD11  | 2.02                     | 0.40              |
| 4:E:169:GLN:O     | 4:E:169:GLN:HG2  | 2.21                     | 0.40              |
| 6:H:33:GLU:O      | 6:H:34:SER:OG    | 2.30                     | 0.40              |
| 6:H:143:LEU:O     | 6:H:143:LEU:HG   | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:N:49:ALA:HB2   | 13:M:84:LEU:O     | 2.21                     | 0.40              |
| 14:R:-6:C:H2'     | 14:R:-5:U:C6      | 2.57                     | 0.40              |
| 1:A:592:ASP:O     | 1:A:593:GLU:C     | 2.60                     | 0.40              |
| 1:A:677:LYS:HB3   | 6:H:91:VAL:H      | 1.86                     | 0.40              |
| 1:A:714:LYS:HB3   | 1:A:714:LYS:HE3   | 1.84                     | 0.40              |
| 1:A:1024:LEU:HB3  | 1:A:1029:THR:HG21 | 2.03                     | 0.40              |
| 1:A:1281:LEU:CD2  | 1:A:1595:LEU:HD11 | 2.51                     | 0.40              |
| 1:A:1357:LYS:NZ   | 1:A:1538:PHE:HE1  | 2.19                     | 0.40              |
| 2:B:95:GLU:HA     | 2:B:95:GLU:OE1    | 2.21                     | 0.40              |
| 2:B:1045:LEU:HD23 | 2:B:1054:LEU:HD13 | 2.04                     | 0.40              |
| 3:C:45:PHE:CZ     | 9:K:106:VAL:HG13  | 2.56                     | 0.40              |
| 4:E:156:VAL:O     | 4:E:160:LEU:HG    | 2.21                     | 0.40              |
| 1:A:32:SER:HB2    | 1:A:80:HIS:CE1    | 2.57                     | 0.40              |
| 1:A:305:PRO:HG3   | 2:B:1125:ALA:HB2  | 2.02                     | 0.40              |
| 1:A:436:ARG:O     | 2:B:1062:SER:HB3  | 2.21                     | 0.40              |
| 1:A:448:ASP:O     | 1:A:449:MET:CB    | 2.69                     | 0.40              |
| 1:A:585:TYR:O     | 1:A:586:ASN:HB3   | 2.21                     | 0.40              |
| 1:A:915:LEU:CD1   | 1:A:952:THR:HA    | 2.51                     | 0.40              |
| 1:A:1557:LYS:O    | 1:A:1584:ASN:ND2  | 2.53                     | 0.40              |
| 2:B:15:SER:O      | 2:B:723:ARG:NH2   | 2.55                     | 0.40              |
| 2:B:46:PHE:CE1    | 2:B:50:VAL:HG11   | 2.56                     | 0.40              |
| 2:B:224:MET:HE2   | 2:B:224:MET:HB2   | 1.86                     | 0.40              |
| 2:B:1101:CYS:O    | 2:B:1101:CYS:SG   | 2.79                     | 0.40              |
| 6:H:43:VAL:HG23   | 6:H:90:TYR:CE2    | 2.57                     | 0.40              |
| 11:N:131:GLN:HB2  | 11:N:134:PRO:HB3  | 2.02                     | 0.40              |
| 13:M:26:VAL:CG1   | 13:M:60:LEU:HD21  | 2.52                     | 0.40              |
| 1:A:473:THR:HB    | 1:A:474:PRO:CD    | 2.52                     | 0.40              |
| 1:A:651:GLU:HG3   | 9:K:60:MET:CE     | 2.51                     | 0.40              |
| 1:A:740:ARG:O     | 1:A:741:GLU:HB2   | 2.22                     | 0.40              |
| 1:A:1034:PRO:O    | 1:A:1035:LYS:CB   | 2.69                     | 0.40              |
| 1:A:1156:PHE:HE1  | 1:A:1198:LEU:CD2  | 2.35                     | 0.40              |
| 2:B:166:MET:SD    | 2:B:166:MET:N     | 2.94                     | 0.40              |
| 6:H:88:PHE:HA     | 6:H:146:LYS:HB2   | 2.03                     | 0.40              |
| 13:M:28:PHE:HB2   | 13:M:31:GLY:O     | 2.20                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 1455/1719 (85%) | 1310 (90%) | 138 (10%) | 7 (0%)   | 29          | 61  |
| 2   | B     | 1119/1135 (99%) | 1019 (91%) | 100 (9%)  | 0        | 100         | 100 |
| 3   | C     | 335/346 (97%)   | 313 (93%)  | 22 (7%)   | 0        | 100         | 100 |
| 4   | E     | 195/210 (93%)   | 185 (95%)  | 10 (5%)   | 0        | 100         | 100 |
| 5   | F     | 74/127 (58%)    | 71 (96%)   | 3 (4%)    | 0        | 100         | 100 |
| 6   | H     | 144/150 (96%)   | 130 (90%)  | 14 (10%)  | 0        | 100         | 100 |
| 7   | I     | 58/126 (46%)    | 43 (74%)   | 13 (22%)  | 2 (3%)   | 3           | 15  |
| 8   | J     | 62/67 (92%)     | 58 (94%)   | 4 (6%)    | 0        | 100         | 100 |
| 9   | K     | 106/133 (80%)   | 96 (91%)   | 9 (8%)    | 1 (1%)   | 17          | 48  |
| 10  | L     | 43/58 (74%)     | 37 (86%)   | 6 (14%)   | 0        | 100         | 100 |
| 11  | N     | 149/510 (29%)   | 134 (90%)  | 13 (9%)   | 2 (1%)   | 12          | 37  |
| 12  | G     | 153/338 (45%)   | 139 (91%)  | 13 (8%)   | 1 (1%)   | 22          | 54  |
| 13  | M     | 108/419 (26%)   | 106 (98%)  | 1 (1%)    | 1 (1%)   | 17          | 48  |
| All | All   | 4001/5338 (75%) | 3641 (91%) | 346 (9%)  | 14 (0%)  | 44          | 71  |

All (14) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 214  | VAL  |
| 1   | A     | 1605 | ILE  |
| 11  | N     | 156  | PRO  |
| 13  | M     | 37   | GLY  |
| 12  | G     | 102  | LEU  |
| 7   | I     | 19   | PHE  |
| 11  | N     | 132  | PRO  |
| 1   | A     | 677  | LYS  |
| 1   | A     | 719  | GLU  |
| 7   | I     | 18   | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 22  | ALA  |
| 1   | A     | 206 | PRO  |
| 9   | K     | 24  | LYS  |
| 1   | A     | 311 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | A     | 1295/1503 (86%) | 1217 (94%) | 78 (6%)  | 19          | 49  |
| 2   | B     | 982/992 (99%)   | 913 (93%)  | 69 (7%)  | 15          | 41  |
| 3   | C     | 296/302 (98%)   | 275 (93%)  | 21 (7%)  | 14          | 40  |
| 4   | E     | 183/192 (95%)   | 181 (99%)  | 2 (1%)   | 73          | 92  |
| 5   | F     | 66/111 (60%)    | 66 (100%)  | 0        | 100         | 100 |
| 6   | H     | 129/131 (98%)   | 126 (98%)  | 3 (2%)   | 50          | 80  |
| 7   | I     | 53/111 (48%)    | 53 (100%)  | 0        | 100         | 100 |
| 8   | J     | 53/56 (95%)     | 50 (94%)   | 3 (6%)   | 20          | 51  |
| 9   | K     | 96/119 (81%)    | 94 (98%)   | 2 (2%)   | 53          | 81  |
| 10  | L     | 42/55 (76%)     | 41 (98%)   | 1 (2%)   | 49          | 79  |
| 11  | N     | 119/427 (28%)   | 114 (96%)  | 5 (4%)   | 30          | 63  |
| 12  | G     | 135/288 (47%)   | 132 (98%)  | 3 (2%)   | 52          | 81  |
| 13  | M     | 94/366 (26%)    | 88 (94%)   | 6 (6%)   | 17          | 45  |
| All | All   | 3543/4653 (76%) | 3350 (95%) | 193 (5%) | 26          | 54  |

All (193) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 16  | SER  |
| 1   | A     | 19  | MET  |
| 1   | A     | 65  | SER  |
| 1   | A     | 82  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 83  | LEU  |
| 1   | A     | 85  | LEU  |
| 1   | A     | 86  | THR  |
| 1   | A     | 159 | GLU  |
| 1   | A     | 200 | MET  |
| 1   | A     | 204 | ARG  |
| 1   | A     | 205 | CYS  |
| 1   | A     | 206 | PRO  |
| 1   | A     | 209 | LYS  |
| 1   | A     | 217 | LYS  |
| 1   | A     | 292 | PHE  |
| 1   | A     | 295 | SER  |
| 1   | A     | 303 | VAL  |
| 1   | A     | 304 | VAL  |
| 1   | A     | 312 | VAL  |
| 1   | A     | 315 | LEU  |
| 1   | A     | 318 | GLN  |
| 1   | A     | 319 | MET  |
| 1   | A     | 324 | GLN  |
| 1   | A     | 341 | LEU  |
| 1   | A     | 348 | GLU  |
| 1   | A     | 381 | GLN  |
| 1   | A     | 383 | LEU  |
| 1   | A     | 406 | MET  |
| 1   | A     | 408 | LYS  |
| 1   | A     | 409 | LEU  |
| 1   | A     | 410 | MET  |
| 1   | A     | 412 | ASP  |
| 1   | A     | 453 | THR  |
| 1   | A     | 454 | ASN  |
| 1   | A     | 484 | VAL  |
| 1   | A     | 535 | THR  |
| 1   | A     | 536 | LYS  |
| 1   | A     | 550 | LEU  |
| 1   | A     | 553 | GLN  |
| 1   | A     | 555 | THR  |
| 1   | A     | 557 | HIS  |
| 1   | A     | 635 | MET  |
| 1   | A     | 676 | LEU  |
| 1   | A     | 680 | PRO  |
| 1   | A     | 701 | ILE  |
| 1   | A     | 718 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 833  | LEU  |
| 1   | A     | 839  | TYR  |
| 1   | A     | 878  | LYS  |
| 1   | A     | 885  | LEU  |
| 1   | A     | 888  | GLN  |
| 1   | A     | 891  | GLU  |
| 1   | A     | 981  | LYS  |
| 1   | A     | 1045 | GLU  |
| 1   | A     | 1051 | GLN  |
| 1   | A     | 1057 | LEU  |
| 1   | A     | 1104 | LYS  |
| 1   | A     | 1110 | ARG  |
| 1   | A     | 1145 | PRO  |
| 1   | A     | 1184 | LYS  |
| 1   | A     | 1186 | GLU  |
| 1   | A     | 1263 | MET  |
| 1   | A     | 1266 | VAL  |
| 1   | A     | 1269 | LEU  |
| 1   | A     | 1272 | LYS  |
| 1   | A     | 1288 | VAL  |
| 1   | A     | 1289 | CYS  |
| 1   | A     | 1313 | GLN  |
| 1   | A     | 1316 | GLN  |
| 1   | A     | 1317 | LEU  |
| 1   | A     | 1340 | ARG  |
| 1   | A     | 1505 | VAL  |
| 1   | A     | 1507 | GLU  |
| 1   | A     | 1508 | ILE  |
| 1   | A     | 1509 | HIS  |
| 1   | A     | 1556 | THR  |
| 1   | A     | 1603 | ASN  |
| 1   | A     | 1677 | SER  |
| 2   | B     | 6    | ARG  |
| 2   | B     | 26   | ILE  |
| 2   | B     | 29   | GLU  |
| 2   | B     | 31   | GLN  |
| 2   | B     | 35   | LEU  |
| 2   | B     | 71   | GLU  |
| 2   | B     | 73   | ILE  |
| 2   | B     | 74   | SER  |
| 2   | B     | 76   | THR  |
| 2   | B     | 79   | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 111 | ARG  |
| 2   | B     | 222 | VAL  |
| 2   | B     | 224 | MET  |
| 2   | B     | 231 | ASN  |
| 2   | B     | 235 | MET  |
| 2   | B     | 254 | LYS  |
| 2   | B     | 260 | SER  |
| 2   | B     | 267 | GLU  |
| 2   | B     | 273 | GLU  |
| 2   | B     | 276 | SER  |
| 2   | B     | 278 | LEU  |
| 2   | B     | 289 | VAL  |
| 2   | B     | 290 | MET  |
| 2   | B     | 292 | GLU  |
| 2   | B     | 314 | VAL  |
| 2   | B     | 317 | TRP  |
| 2   | B     | 318 | TYR  |
| 2   | B     | 325 | GLU  |
| 2   | B     | 327 | LEU  |
| 2   | B     | 330 | GLN  |
| 2   | B     | 337 | LYS  |
| 2   | B     | 338 | SER  |
| 2   | B     | 345 | MET  |
| 2   | B     | 348 | LEU  |
| 2   | B     | 361 | CYS  |
| 2   | B     | 365 | ASN  |
| 2   | B     | 429 | PRO  |
| 2   | B     | 430 | PHE  |
| 2   | B     | 454 | CYS  |
| 2   | B     | 461 | ASN  |
| 2   | B     | 463 | ILE  |
| 2   | B     | 466 | LEU  |
| 2   | B     | 501 | HIS  |
| 2   | B     | 506 | GLU  |
| 2   | B     | 537 | LEU  |
| 2   | B     | 542 | ILE  |
| 2   | B     | 547 | HIS  |
| 2   | B     | 582 | LYS  |
| 2   | B     | 601 | THR  |
| 2   | B     | 659 | GLN  |
| 2   | B     | 666 | LEU  |
| 2   | B     | 667 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 678  | ASP  |
| 2   | B     | 680  | ASN  |
| 2   | B     | 728  | ASP  |
| 2   | B     | 755  | ASP  |
| 2   | B     | 792  | LEU  |
| 2   | B     | 793  | VAL  |
| 2   | B     | 797  | LYS  |
| 2   | B     | 828  | TYR  |
| 2   | B     | 859  | THR  |
| 2   | B     | 864  | PHE  |
| 2   | B     | 866  | CYS  |
| 2   | B     | 1010 | PHE  |
| 2   | B     | 1012 | VAL  |
| 2   | B     | 1015 | THR  |
| 2   | B     | 1077 | LEU  |
| 2   | B     | 1081 | LEU  |
| 2   | B     | 1106 | THR  |
| 3   | C     | 21   | VAL  |
| 3   | C     | 22   | ARG  |
| 3   | C     | 55   | HIS  |
| 3   | C     | 58   | GLU  |
| 3   | C     | 96   | ASN  |
| 3   | C     | 114  | PRO  |
| 3   | C     | 133  | THR  |
| 3   | C     | 134  | GLU  |
| 3   | C     | 135  | ILE  |
| 3   | C     | 136  | ASP  |
| 3   | C     | 137  | THR  |
| 3   | C     | 144  | VAL  |
| 3   | C     | 151  | HIS  |
| 3   | C     | 155  | ASP  |
| 3   | C     | 161  | GLU  |
| 3   | C     | 166  | HIS  |
| 3   | C     | 183  | ASP  |
| 3   | C     | 196  | ASP  |
| 3   | C     | 266  | GLU  |
| 3   | C     | 267  | VAL  |
| 3   | C     | 274  | ARG  |
| 4   | E     | 31   | ASP  |
| 4   | E     | 107  | GLN  |
| 6   | H     | 15   | ILE  |
| 6   | H     | 80   | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | H     | 83  | SER  |
| 8   | J     | 5   | VAL  |
| 8   | J     | 9   | THR  |
| 8   | J     | 28  | GLU  |
| 9   | K     | 27  | LEU  |
| 9   | K     | 30  | VAL  |
| 10  | L     | 52  | LEU  |
| 11  | N     | 25  | SER  |
| 11  | N     | 60  | HIS  |
| 11  | N     | 116 | ARG  |
| 11  | N     | 118 | LEU  |
| 11  | N     | 130 | LEU  |
| 12  | G     | 94  | ASP  |
| 12  | G     | 98  | VAL  |
| 12  | G     | 169 | MET  |
| 13  | M     | 33  | LEU  |
| 13  | M     | 35  | SER  |
| 13  | M     | 67  | LEU  |
| 13  | M     | 81  | CYS  |
| 13  | M     | 110 | GLN  |
| 13  | M     | 112 | LEU  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 44  | ASN  |
| 1   | A     | 77  | HIS  |
| 1   | A     | 80  | HIS  |
| 1   | A     | 133 | GLN  |
| 1   | A     | 171 | ASN  |
| 1   | A     | 322 | ASN  |
| 1   | A     | 347 | GLN  |
| 1   | A     | 395 | GLN  |
| 1   | A     | 397 | HIS  |
| 1   | A     | 431 | HIS  |
| 1   | A     | 478 | GLN  |
| 1   | A     | 482 | GLN  |
| 1   | A     | 486 | ASN  |
| 1   | A     | 499 | ASN  |
| 1   | A     | 564 | HIS  |
| 1   | A     | 578 | HIS  |
| 1   | A     | 595 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 617  | GLN  |
| 1   | A     | 632  | GLN  |
| 1   | A     | 652  | HIS  |
| 1   | A     | 728  | ASN  |
| 1   | A     | 753  | HIS  |
| 1   | A     | 790  | GLN  |
| 1   | A     | 847  | GLN  |
| 1   | A     | 850  | HIS  |
| 1   | A     | 859  | ASN  |
| 1   | A     | 918  | GLN  |
| 1   | A     | 1051 | GLN  |
| 1   | A     | 1068 | HIS  |
| 1   | A     | 1076 | GLN  |
| 1   | A     | 1094 | GLN  |
| 1   | A     | 1109 | ASN  |
| 1   | A     | 1118 | GLN  |
| 1   | A     | 1136 | GLN  |
| 1   | A     | 1177 | GLN  |
| 1   | A     | 1295 | GLN  |
| 1   | A     | 1300 | GLN  |
| 1   | A     | 1329 | GLN  |
| 1   | A     | 1579 | ASN  |
| 1   | A     | 1603 | ASN  |
| 1   | A     | 1690 | HIS  |
| 1   | A     | 1717 | GLN  |
| 2   | B     | 18   | HIS  |
| 2   | B     | 30   | GLN  |
| 2   | B     | 31   | GLN  |
| 2   | B     | 97   | ASN  |
| 2   | B     | 147  | ASN  |
| 2   | B     | 150  | ASN  |
| 2   | B     | 219  | HIS  |
| 2   | B     | 223  | ASN  |
| 2   | B     | 313  | ASN  |
| 2   | B     | 415  | ASN  |
| 2   | B     | 473  | HIS  |
| 2   | B     | 501  | HIS  |
| 2   | B     | 523  | GLN  |
| 2   | B     | 547  | HIS  |
| 2   | B     | 690  | GLN  |
| 2   | B     | 694  | GLN  |
| 2   | B     | 709  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 734  | ASN  |
| 2   | B     | 846  | ASN  |
| 2   | B     | 887  | HIS  |
| 2   | B     | 889  | GLN  |
| 2   | B     | 941  | HIS  |
| 2   | B     | 1068 | HIS  |
| 3   | C     | 32   | ASN  |
| 3   | C     | 59   | ASN  |
| 3   | C     | 102  | GLN  |
| 3   | C     | 127  | GLN  |
| 3   | C     | 166  | HIS  |
| 3   | C     | 180  | ASN  |
| 3   | C     | 181  | GLN  |
| 3   | C     | 290  | ASN  |
| 3   | C     | 305  | HIS  |
| 4   | E     | 132  | GLN  |
| 4   | E     | 133  | GLN  |
| 4   | E     | 169  | GLN  |
| 7   | I     | 8    | ASN  |
| 8   | J     | 61   | ASN  |
| 9   | K     | 85   | GLN  |
| 11  | N     | 60   | HIS  |
| 11  | N     | 88   | GLN  |
| 13  | M     | 34   | GLN  |
| 13  | M     | 98   | GLN  |
| 13  | M     | 110  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed  | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------|-------------------|-----------------|
| 14  | R     | 7/8 (87%) | 1 (14%)           | 0               |

All (1) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | R     | -5  | U    |

There are no RNA pucker outliers to report.

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 19  | 2TM  | A     | 2004 | -    | 27,30,30     | 0.83 | 2 (7%)   | 39,47,47    | 0.69 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 19  | 2TM  | A     | 2004 | -    | -       | 4/19/38/38 | 0/2/2/2 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 19  | A     | 2004 | 2TM  | PA-O2A | -2.56 | 1.50        | 1.56     |
| 19  | A     | 2004 | 2TM  | PB-O1B | -2.43 | 1.50        | 1.56     |

There are no bond angle outliers.

There are no chirality outliers.

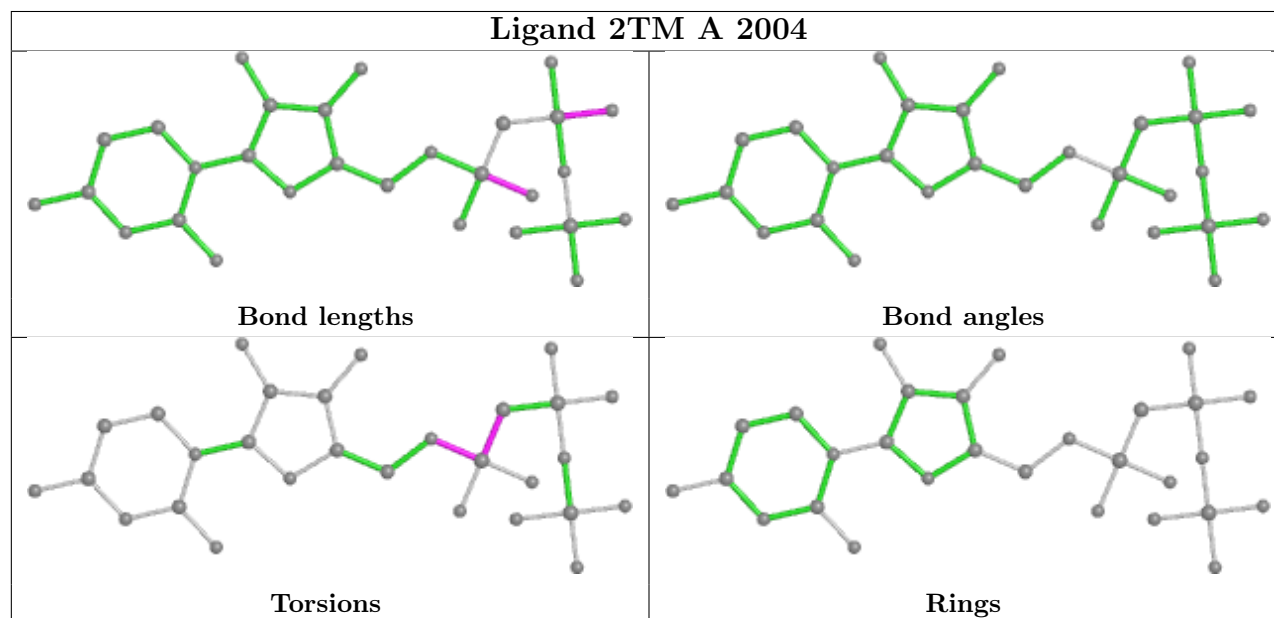
All (4) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 19  | A     | 2004 | 2TM  | PB-C1-PA-O5'  |
| 19  | A     | 2004 | 2TM  | PB-C1-PA-O1A  |
| 19  | A     | 2004 | 2TM  | PB-C1-PA-O2A  |
| 19  | A     | 2004 | 2TM  | C5'-O5'-PA-C1 |

There are no ring outliers.

No monomer is involved in short contacts.

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



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

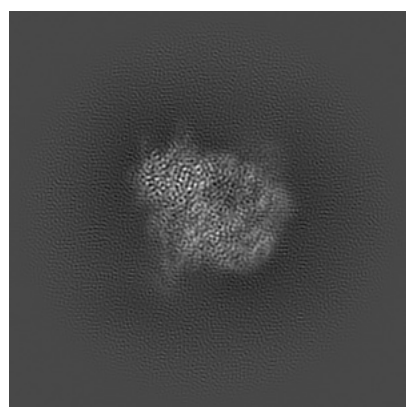
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31876. These allow visual inspection of the internal detail of the map and identification of artifacts.

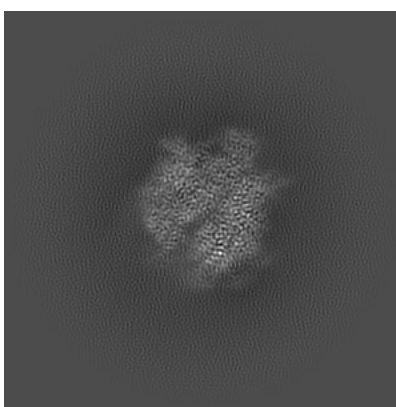
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

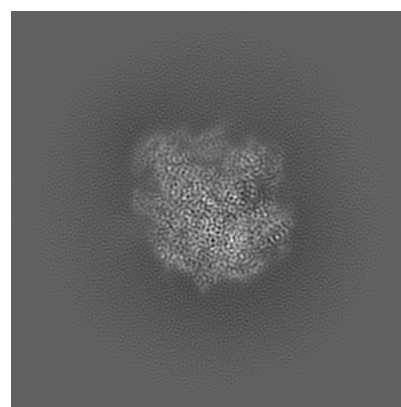
#### 6.1.1 Primary map



X



Y

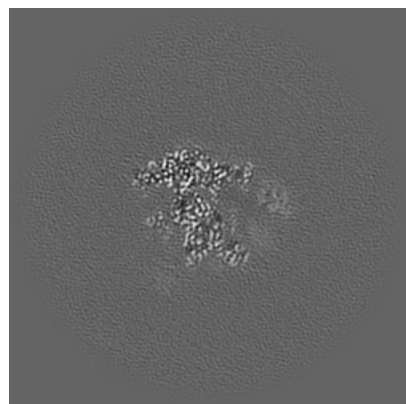


Z

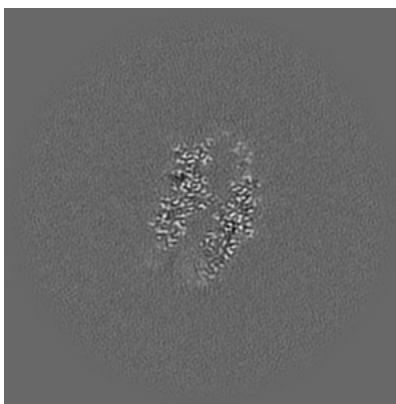
The images above show the map projected in three orthogonal directions.

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

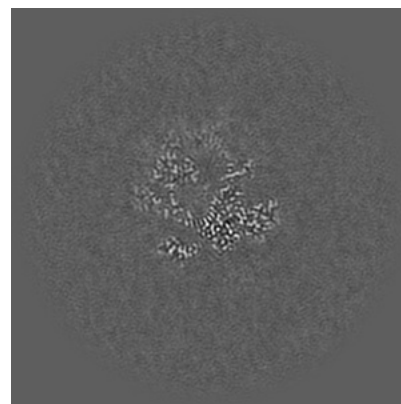
#### 6.2.1 Primary map



X Index: 160



Y Index: 160



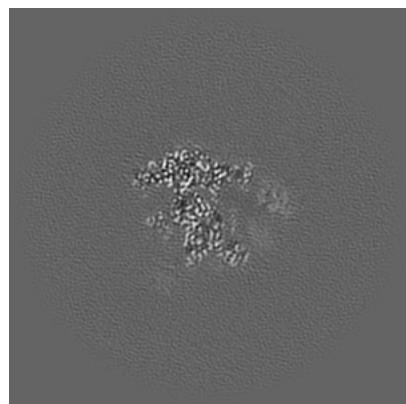
Z Index: 160



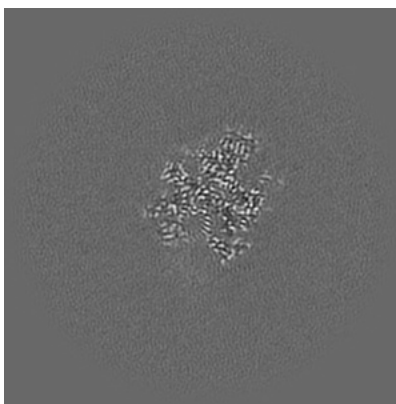
The images above show central slices of the map in three orthogonal directions.

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

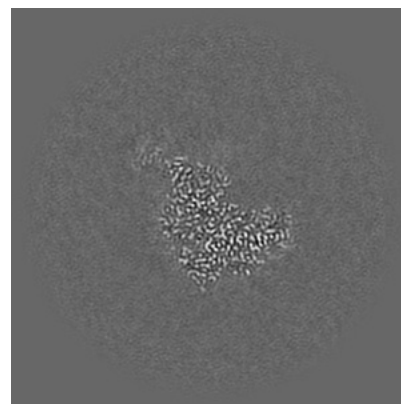
### 6.3.1 Primary map



X Index: 160



Y Index: 146

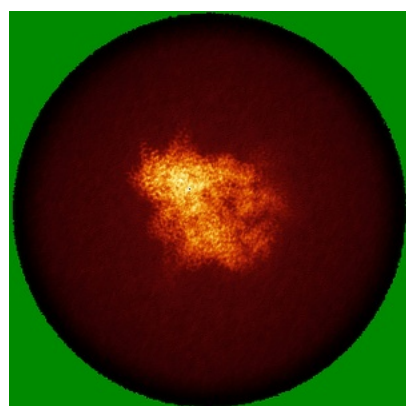


Z Index: 184

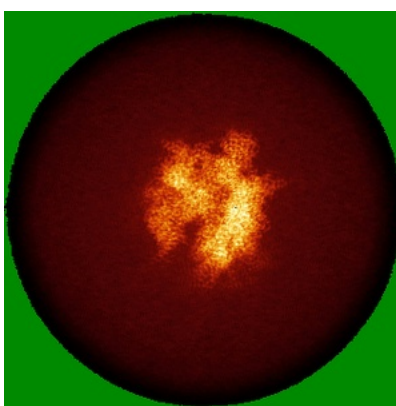
The images above show the largest variance slices of the map in three orthogonal directions.

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

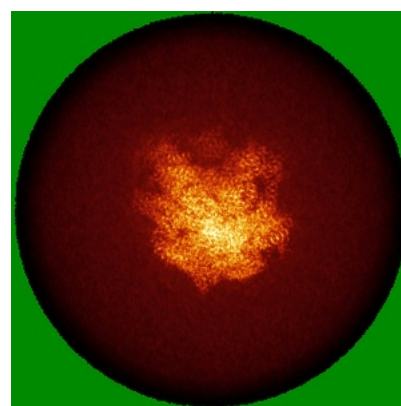
### 6.4.1 Primary map



X



Y

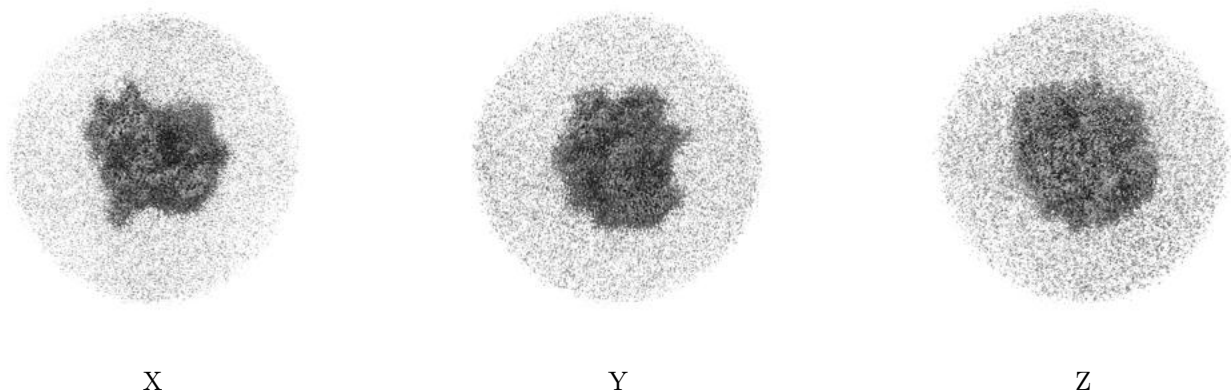


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.351. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

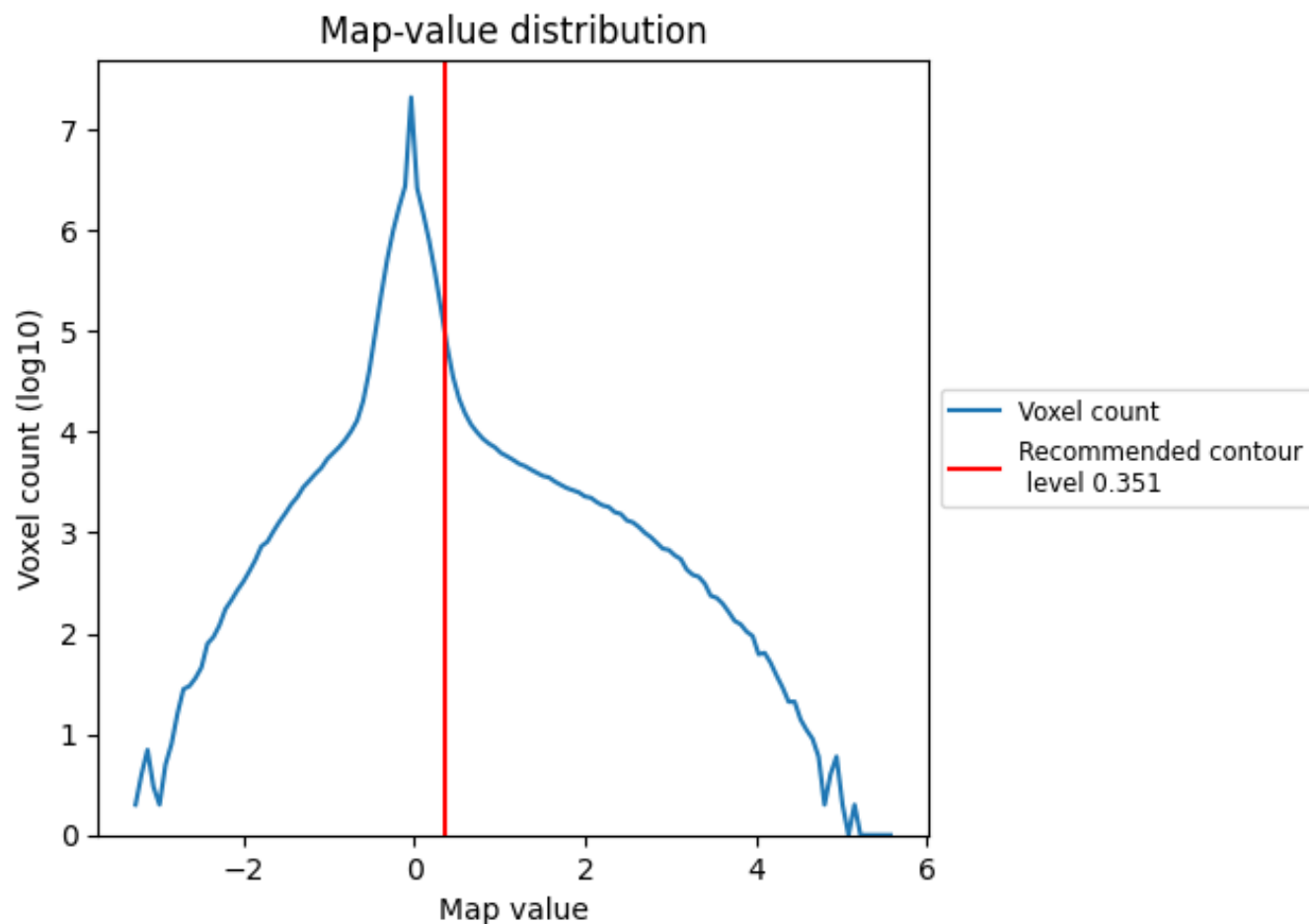
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

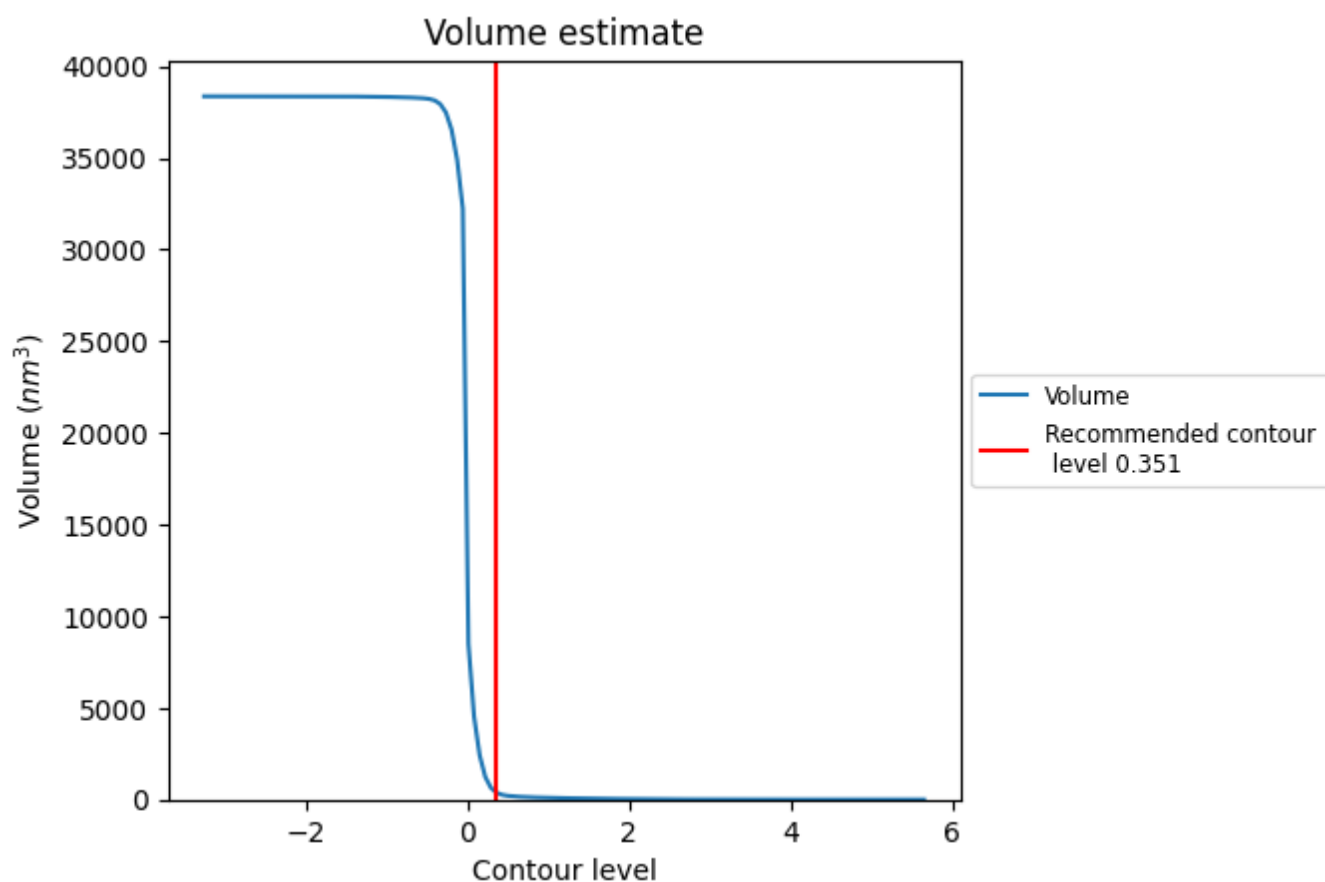
This section contains the results of statistical analysis of the map.

### 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.

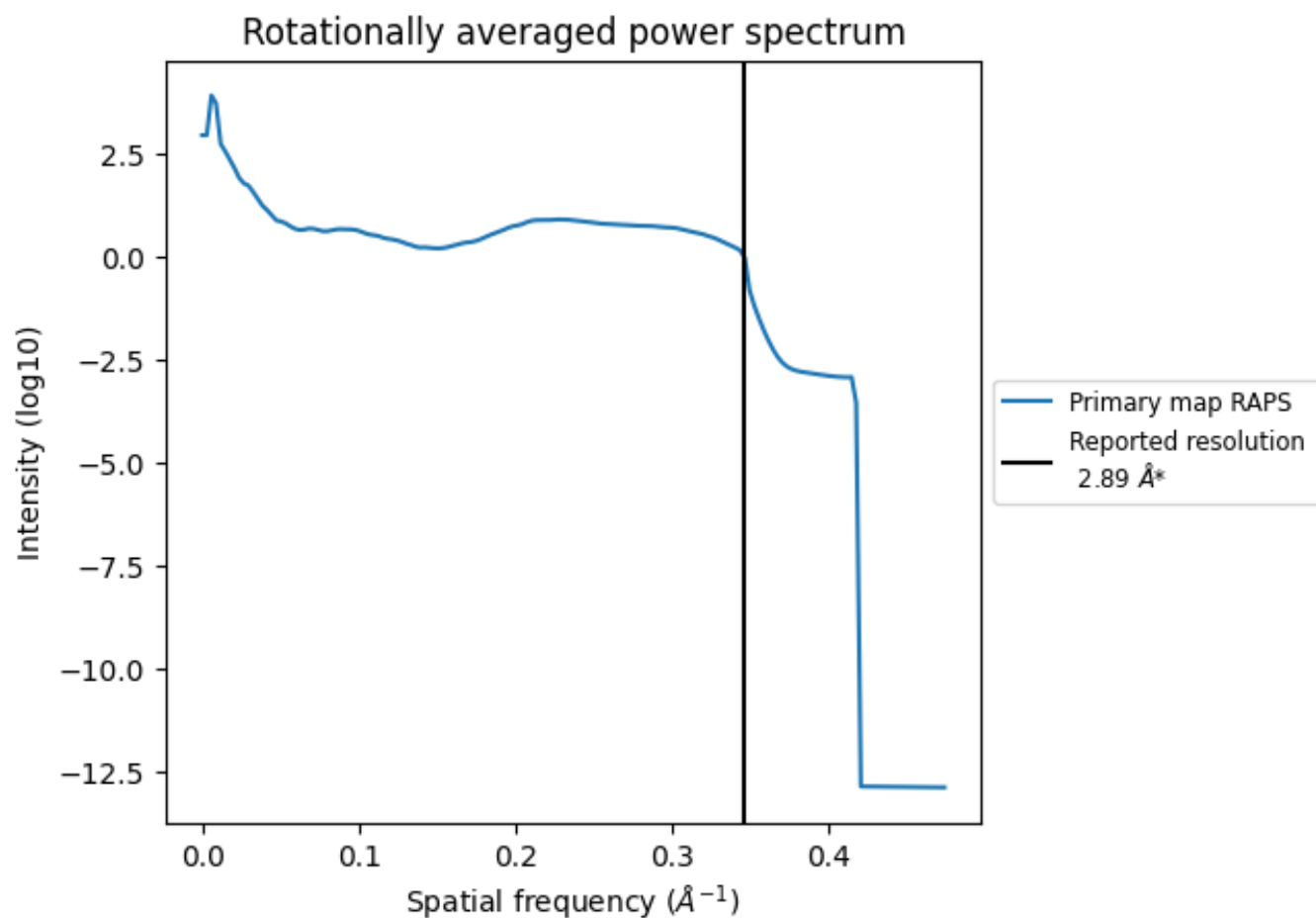
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 392 nm<sup>3</sup>; this corresponds to an approximate mass of 354 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 0.346 Å<sup>-1</sup>

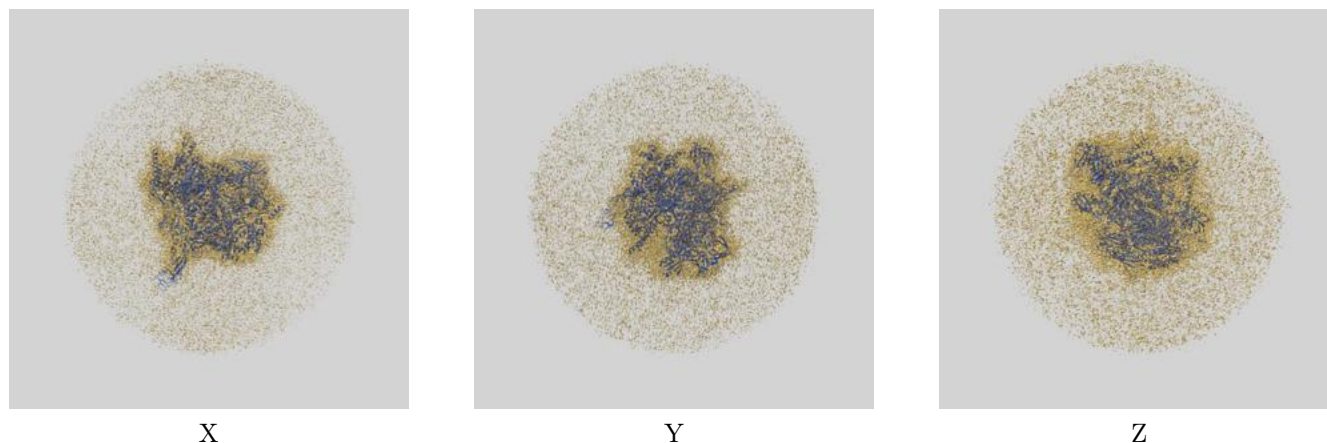
## 8 Fourier-Shell correlation

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

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

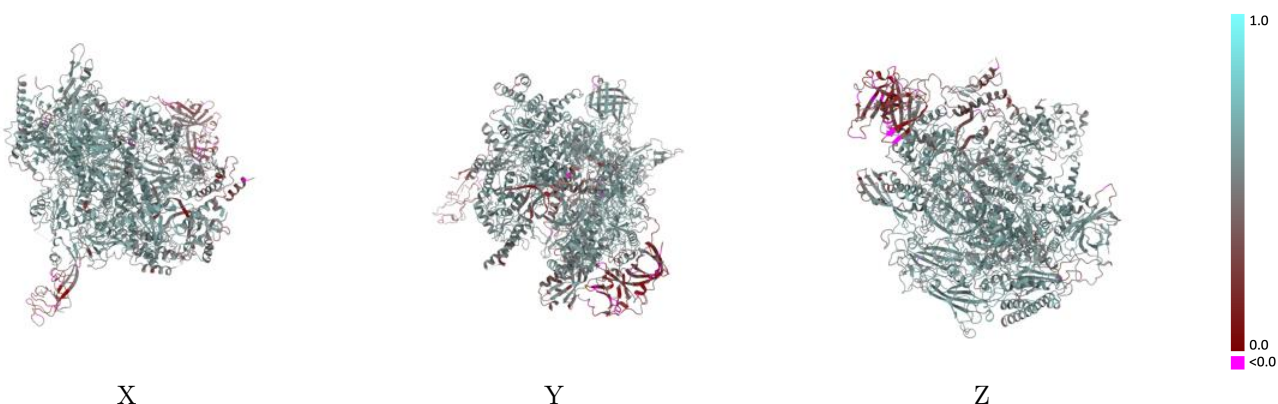
This section contains information regarding the fit between EMDB map EMD-31876 and PDB model 7VBA. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

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



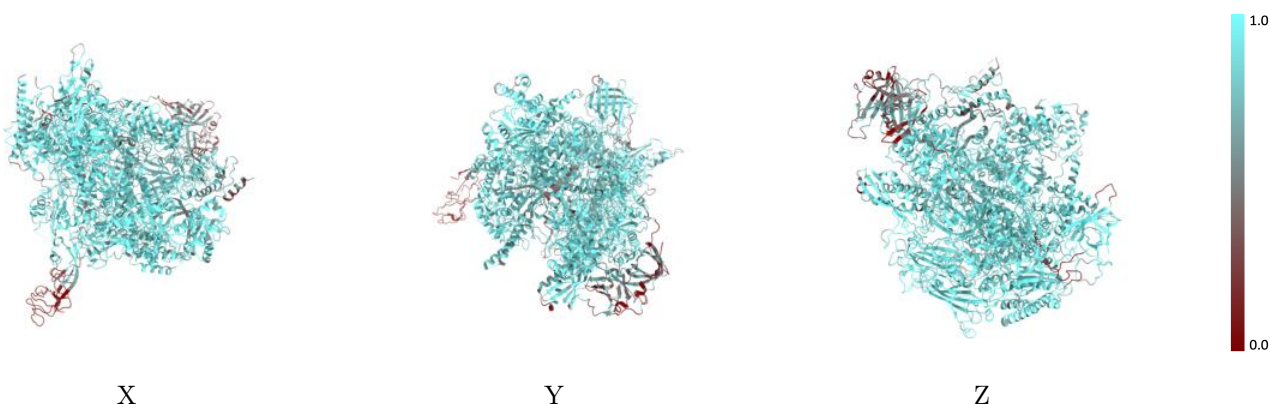
The images above show the 3D surface view of the map at the recommended contour level 0.351 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

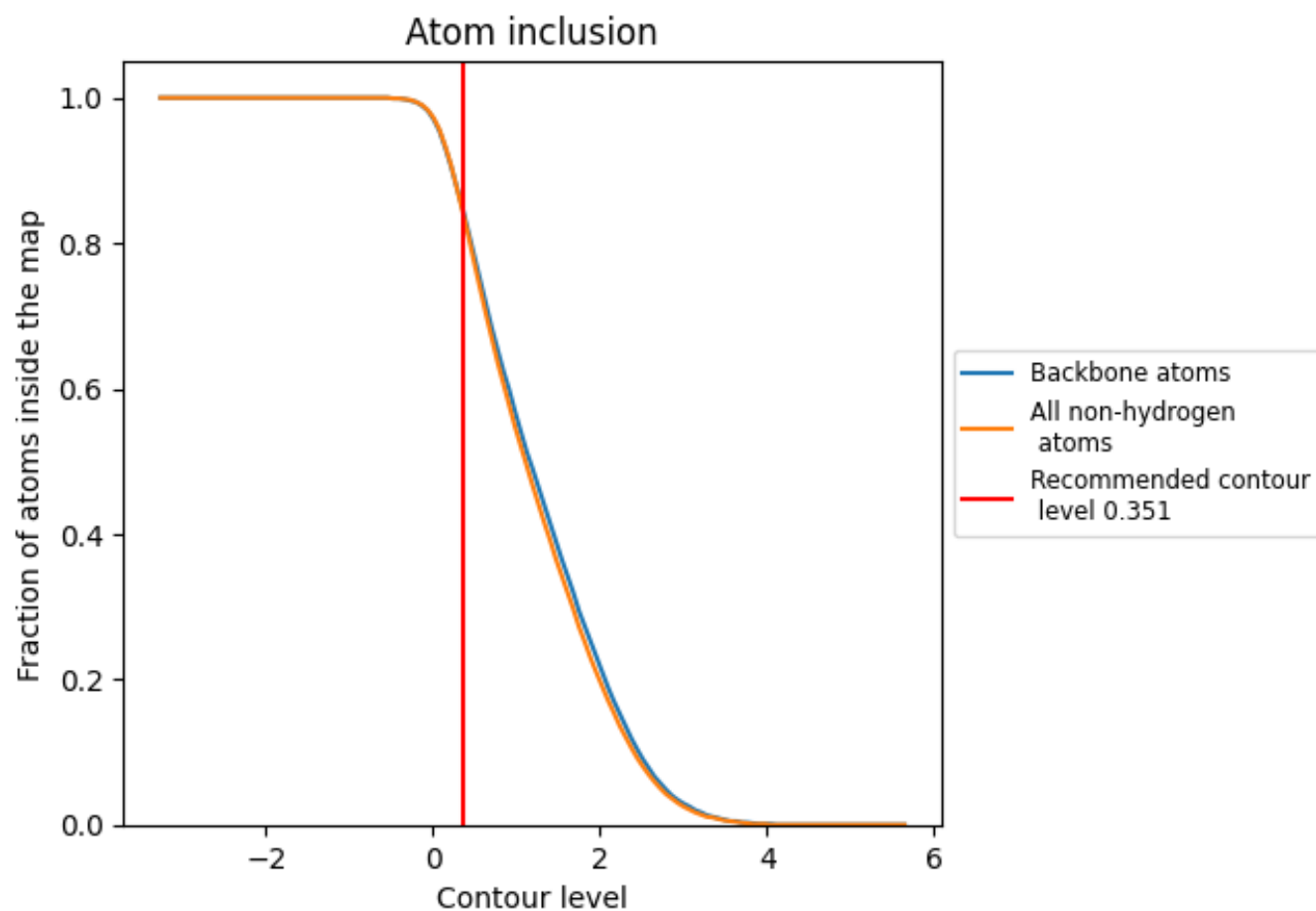
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.351).





































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.351) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8460   |  0.5250   |
| A     |  0.8910   |  0.5470   |
| B     |  0.9240   |  0.5720   |
| C     |  0.8410   |  0.5430   |
| E     |  0.9060   |  0.5570   |
| F     |  0.9360   |  0.5820   |
| G     |  0.3230   |  0.3130   |
| H     |  0.8740   |  0.5410   |
| I     |  0.6300   |  0.3680   |
| J     |  0.9500   |  0.6030   |
| K     |  0.8840   |  0.5490   |
| L     |  0.9150   |  0.5540   |
| M     |  0.5340   |  0.2580   |
| N     |  0.4430   |  0.2390   |
| R     |  0.9170  |  0.5640  |
| T     |  0.8600 |  0.4980 |
| U     |  0.7560 |  0.3880 |

