



## Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 08:49 PM UTC

PDB ID : 8OOU / pdb\_00008oou  
EMDB ID : EMD-17031  
Title : Double-ring nucleocapsid of the Respiratory Syncytial Virus  
Authors : Gonnin, L.; Desfosses, A.; Gutsche, I.  
Deposited on : 2023-04-06  
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

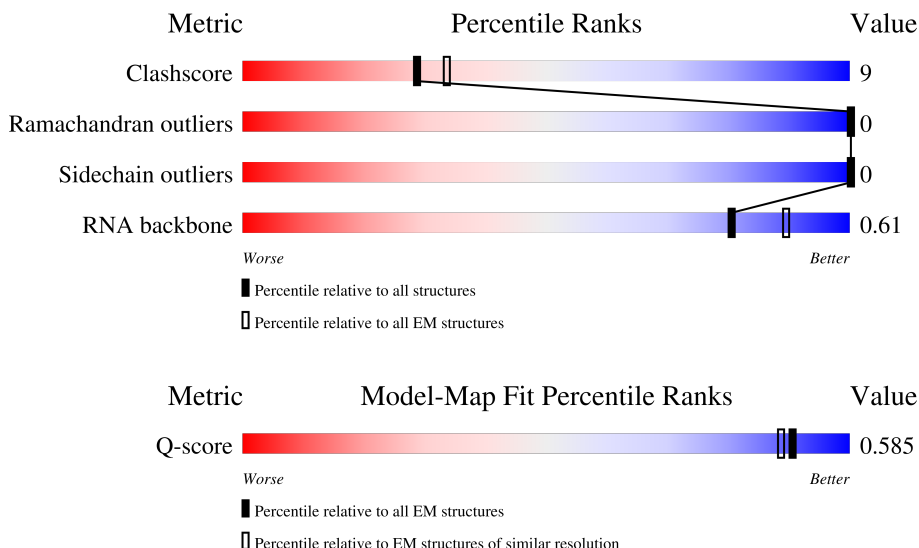
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 13054 ( 2.40 - 3.40 )                                    |

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     | 391    |                  |
| 1   | B     | 391    |                  |
| 1   | C     | 391    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | D     | 391    |                  |
| 1   | E     | 391    |                  |
| 1   | F     | 391    |                  |
| 1   | G     | 391    |                  |
| 1   | H     | 391    |                  |
| 1   | I     | 391    |                  |
| 1   | J     | 391    |                  |
| 1   | K     | 391    |                  |
| 1   | L     | 391    |                  |
| 1   | M     | 391    |                  |
| 1   | N     | 391    |                  |
| 1   | O     | 391    |                  |
| 1   | P     | 391    |                  |
| 1   | Q     | 391    |                  |
| 1   | R     | 391    |                  |
| 1   | S     | 391    |                  |
| 1   | T     | 391    |                  |
| 2   | U     | 70     |                  |
| 2   | e     | 70     |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 61800 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nucleoprotein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | B     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | C     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | D     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | E     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | F     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | G     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | H     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | I     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | J     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | K     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | L     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | M     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | N     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | O     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | P     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | Q     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | R     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | S     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |
| 1   | T     | 378      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 2950  | 1868 | 512 | 554 | 16 |         |       |

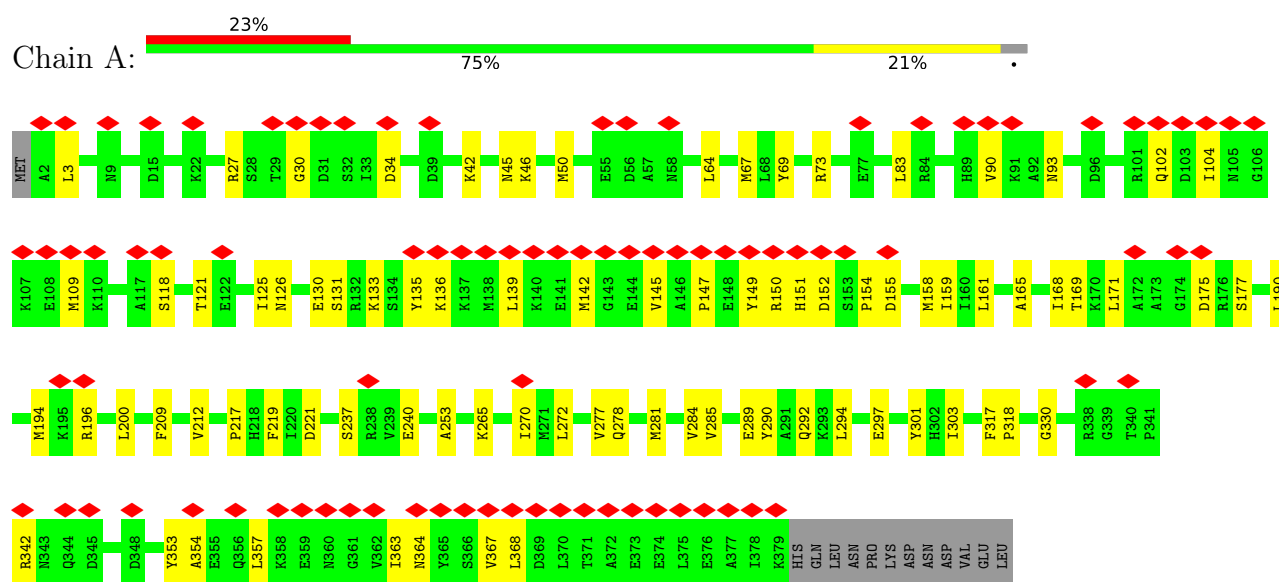
- Molecule 2 is a RNA chain called RNA (70-mer).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | U     | 70       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1400  | 630 | 210 | 490 | 70 |         |       |
| 2   | e     | 70       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1400  | 630 | 210 | 490 | 70 |         |       |

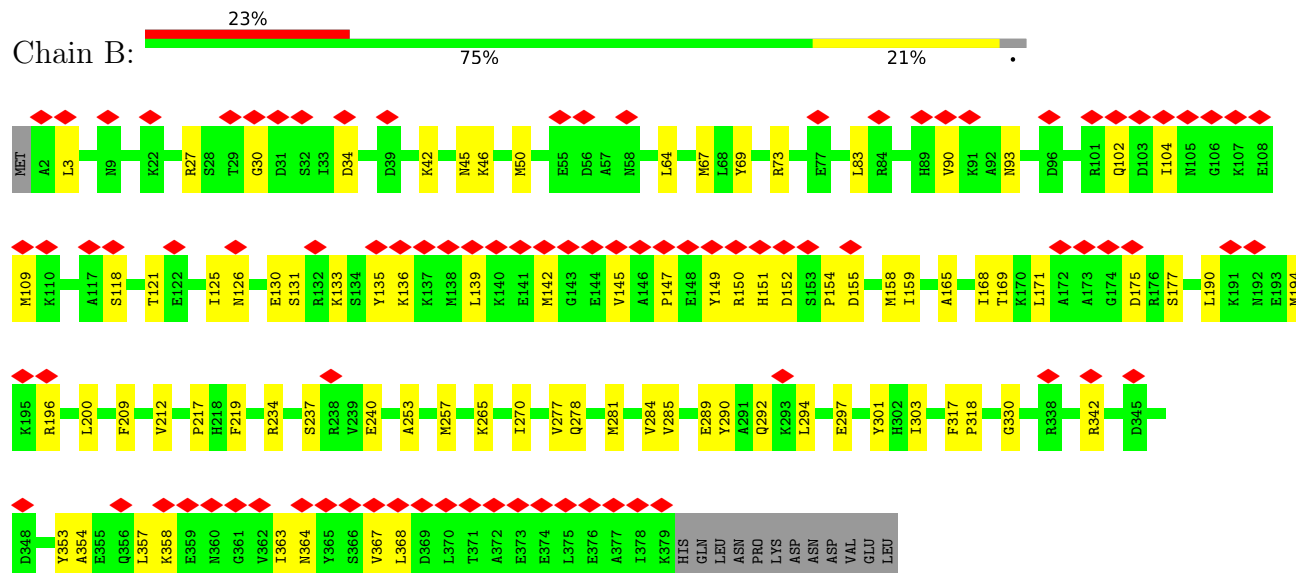
### 3 Residue-property plots

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.

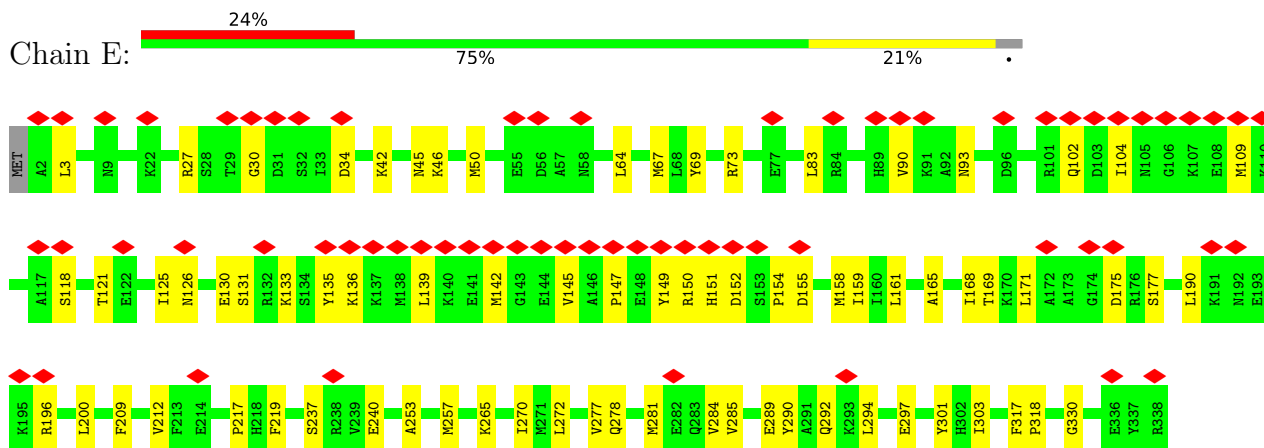
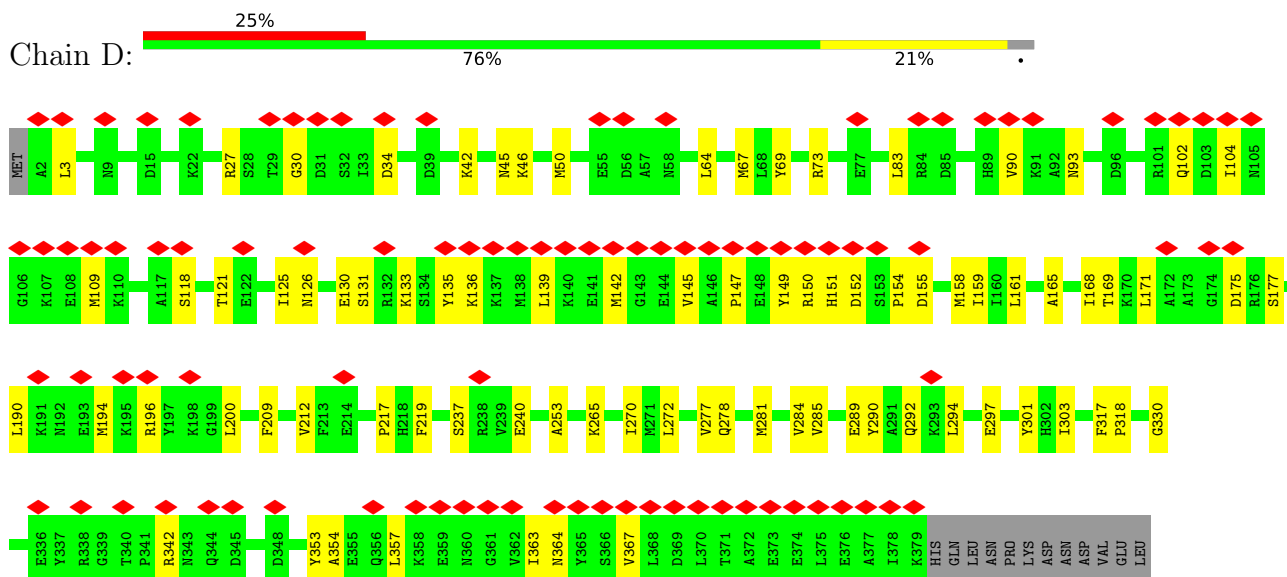
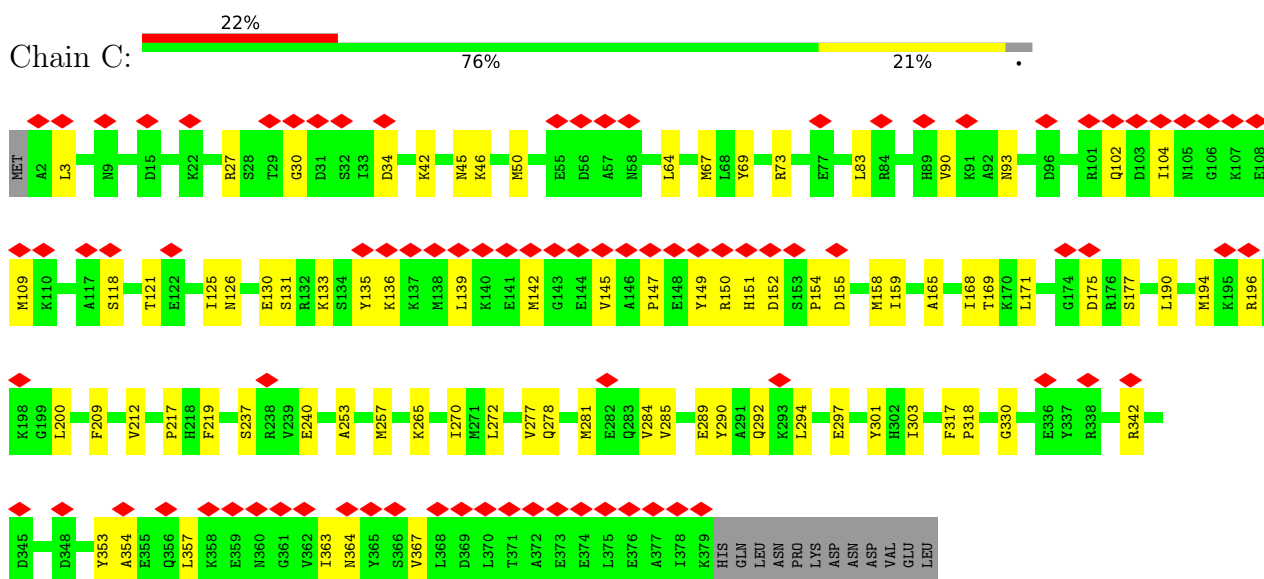
#### • Molecule 1: Nucleoprotein



#### • Molecule 1: Nucleoprotein

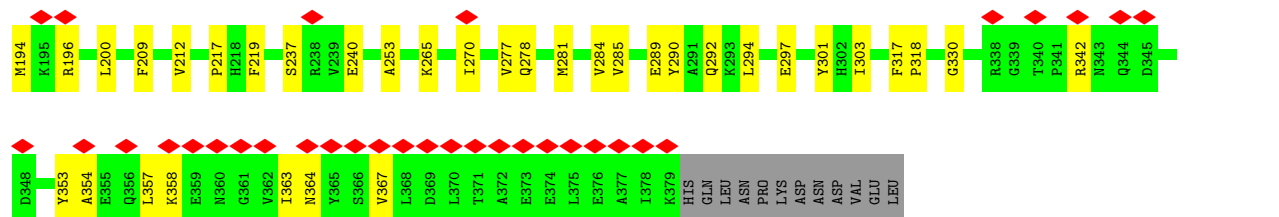
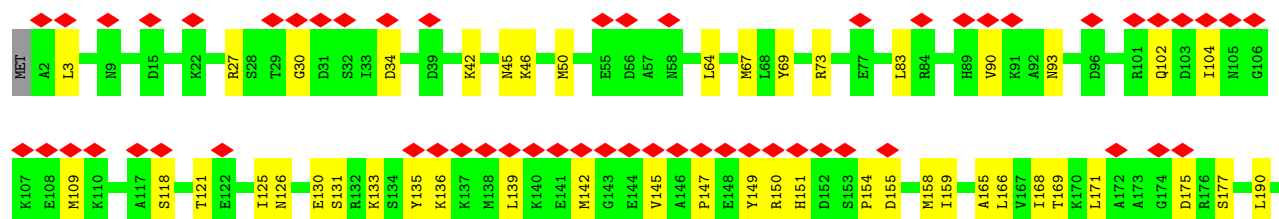
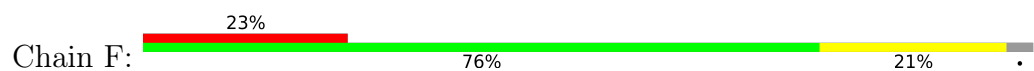


#### • Molecule 1: Nucleoprotein

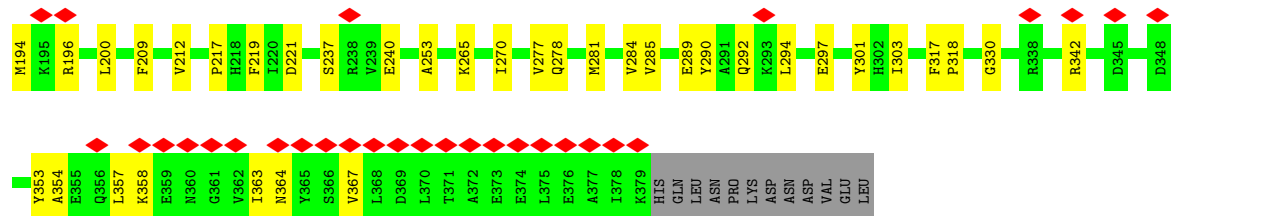
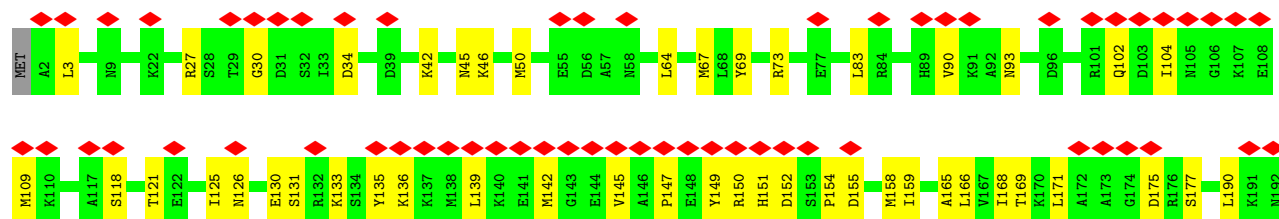
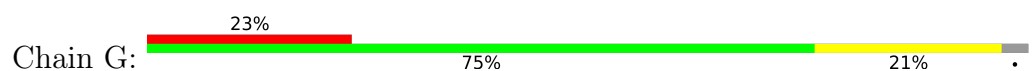




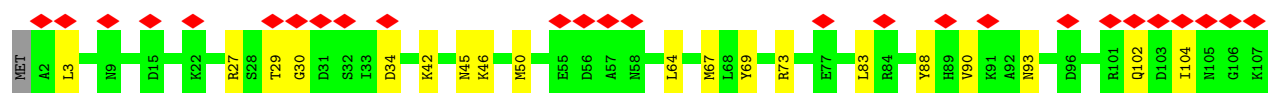
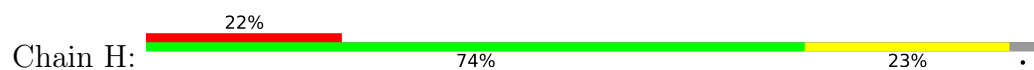
• Molecule 1: Nucleoprotein

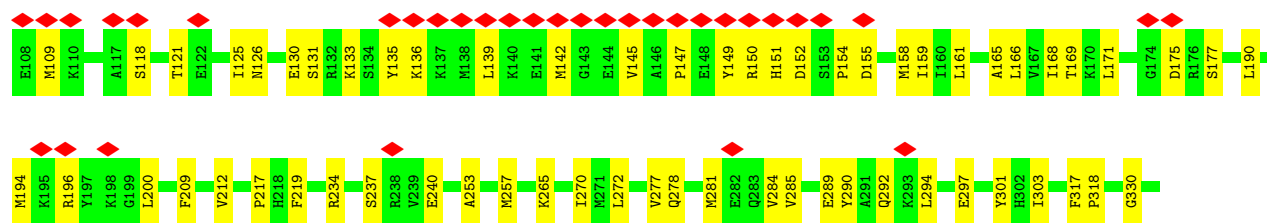


• Molecule 1: Nucleoprotein

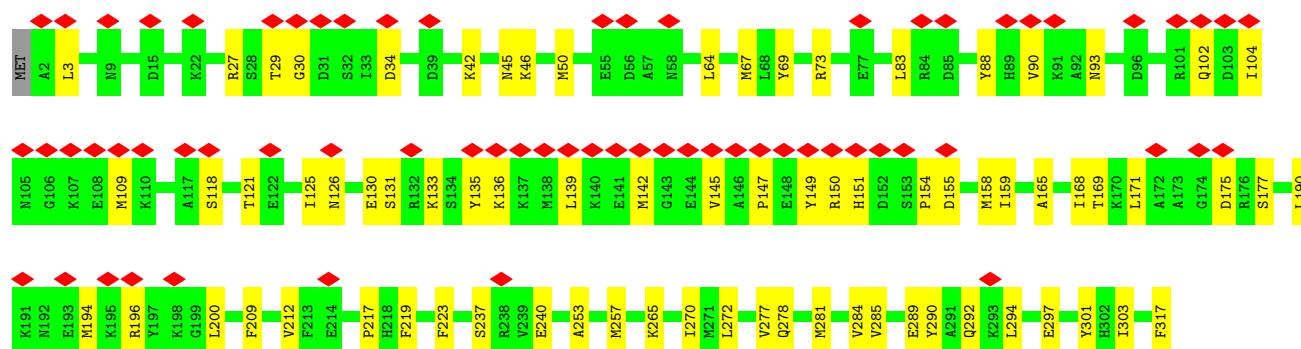
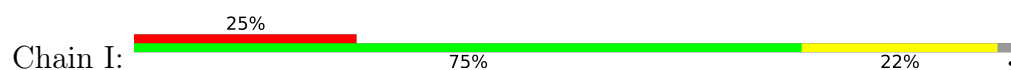


• Molecule 1: Nucleoprotein

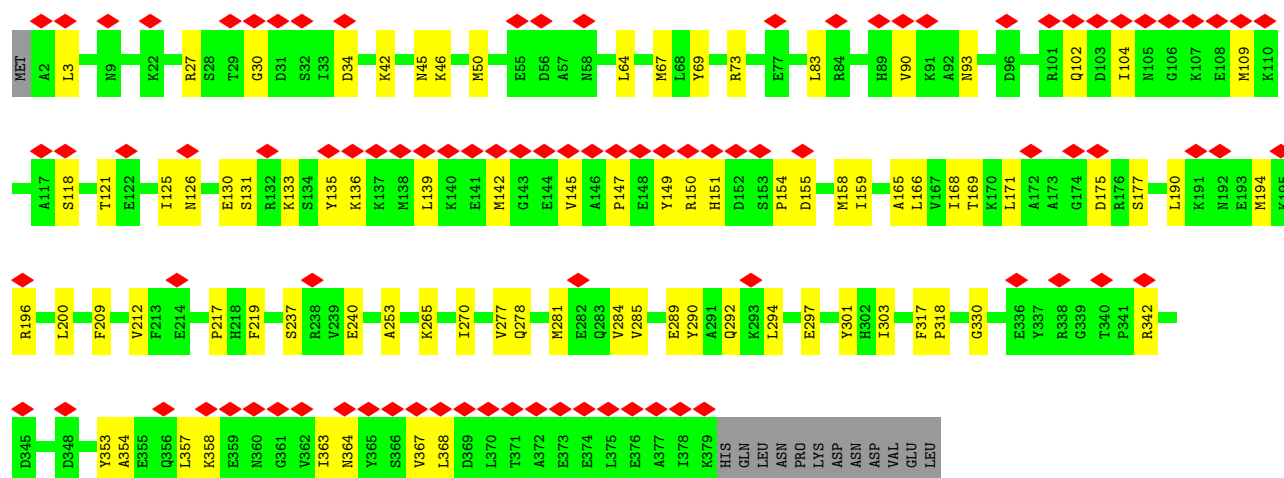
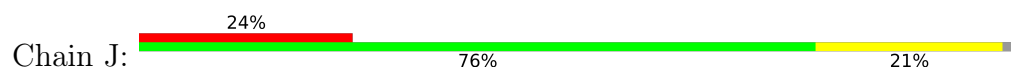




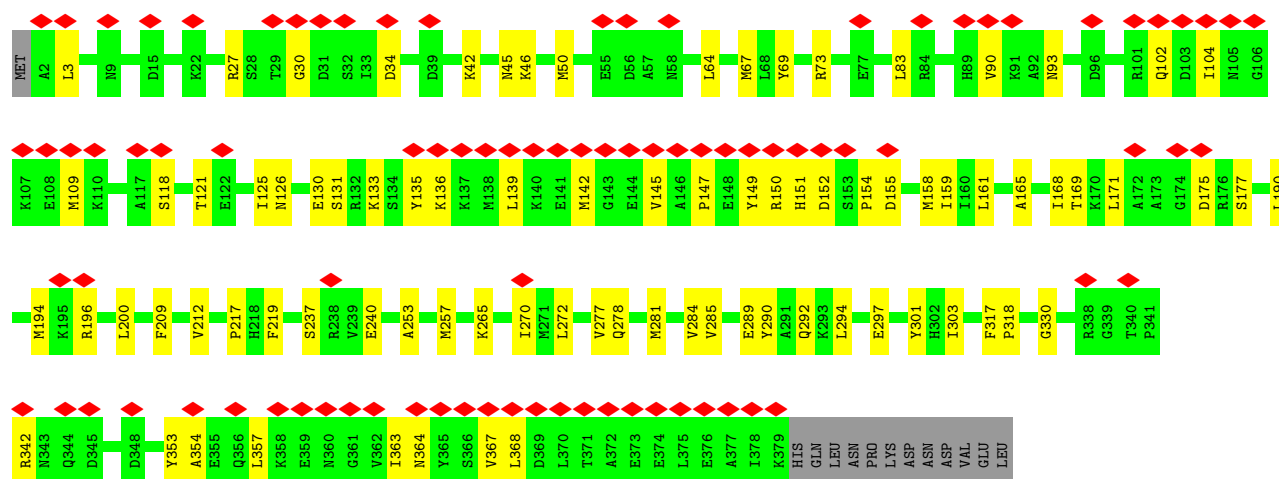
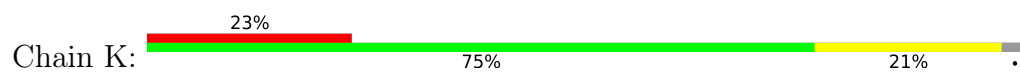
• Molecule 1: Nucleoprotein



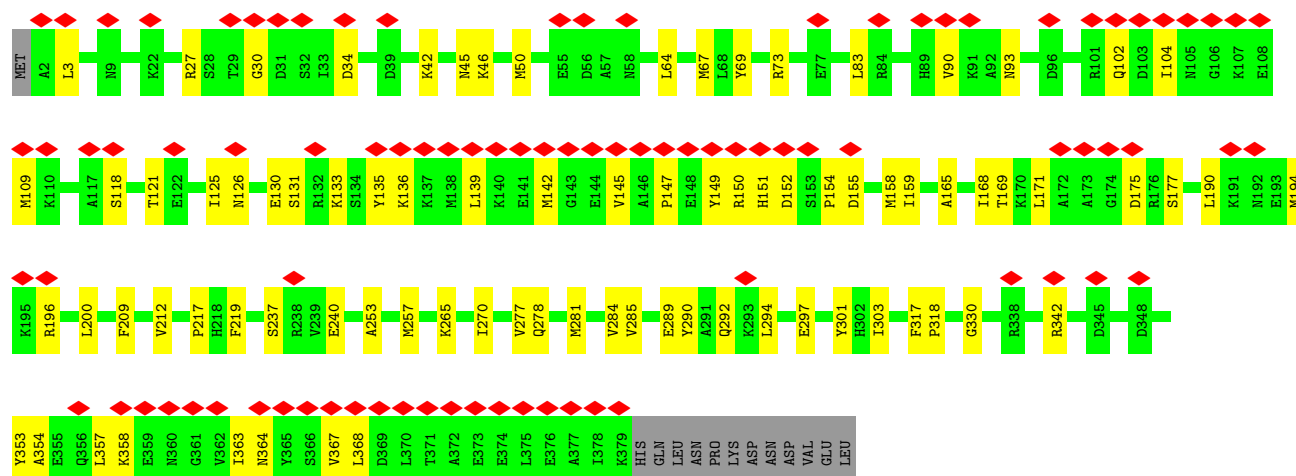
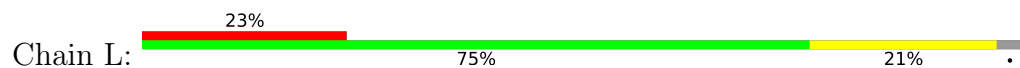
• Molecule 1: Nucleoprotein



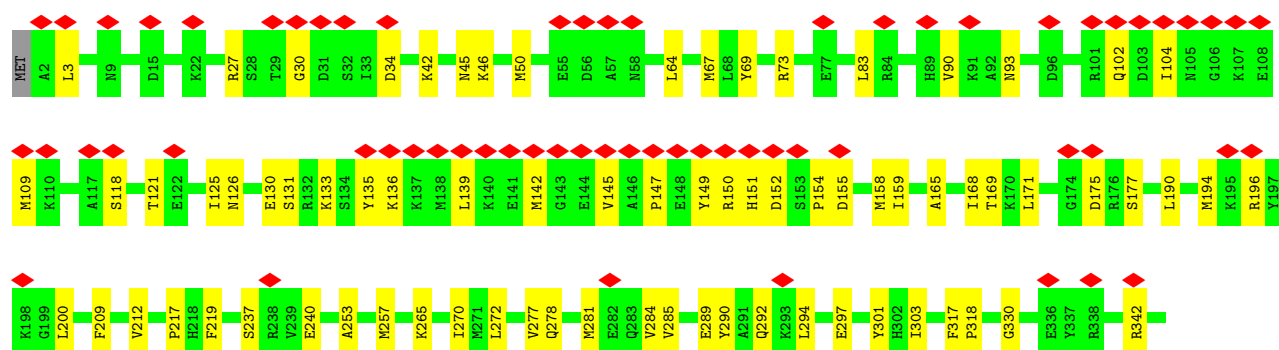
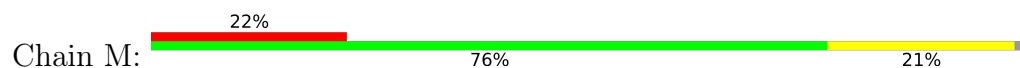
• Molecule 1: Nucleoprotein

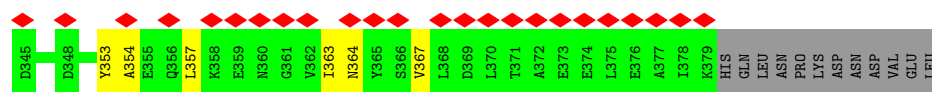


• Molecule 1: Nucleoprotein

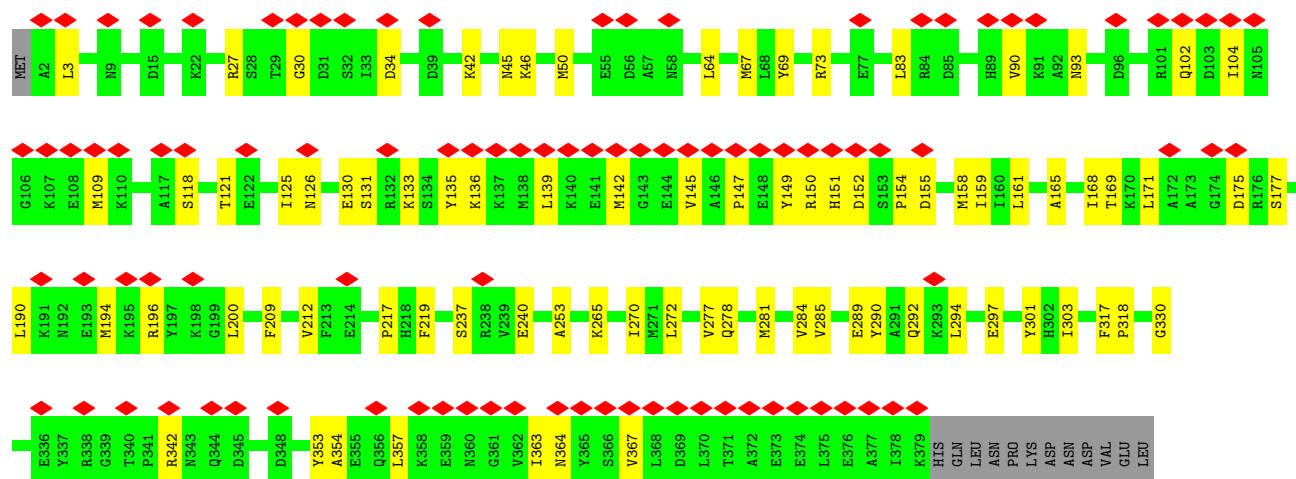
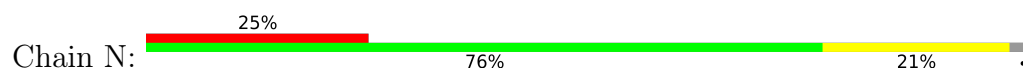


• Molecule 1: Nucleoprotein

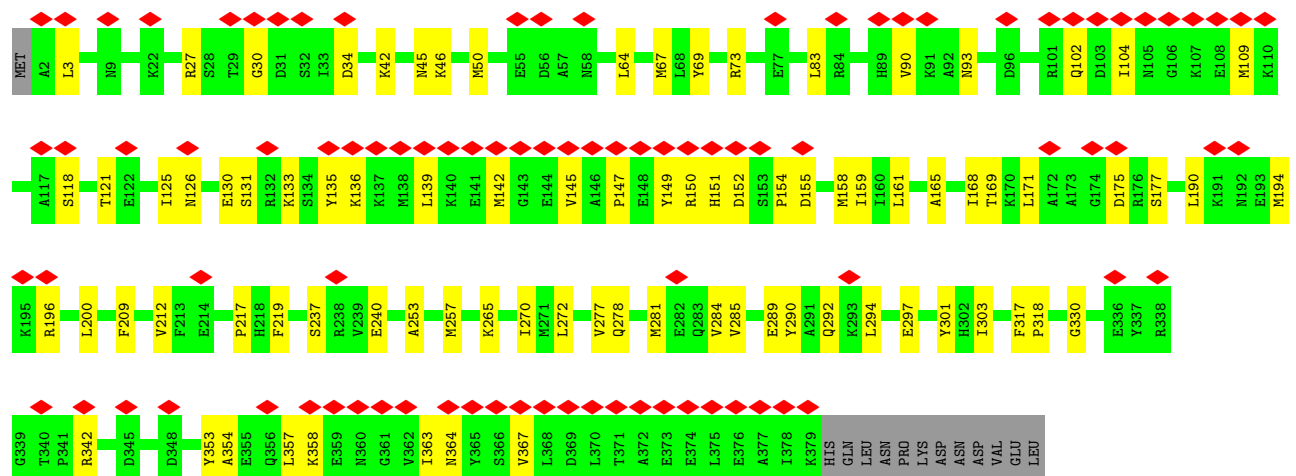
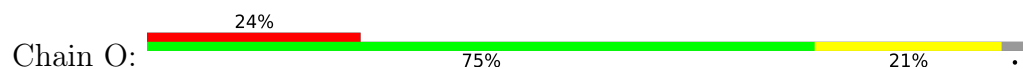




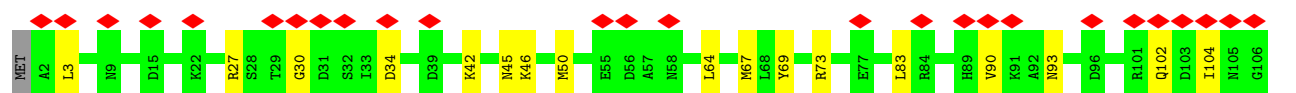
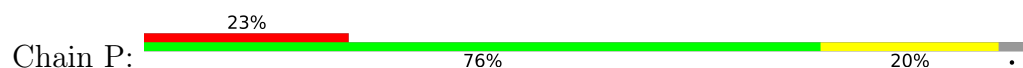
• Molecule 1: Nucleoprotein

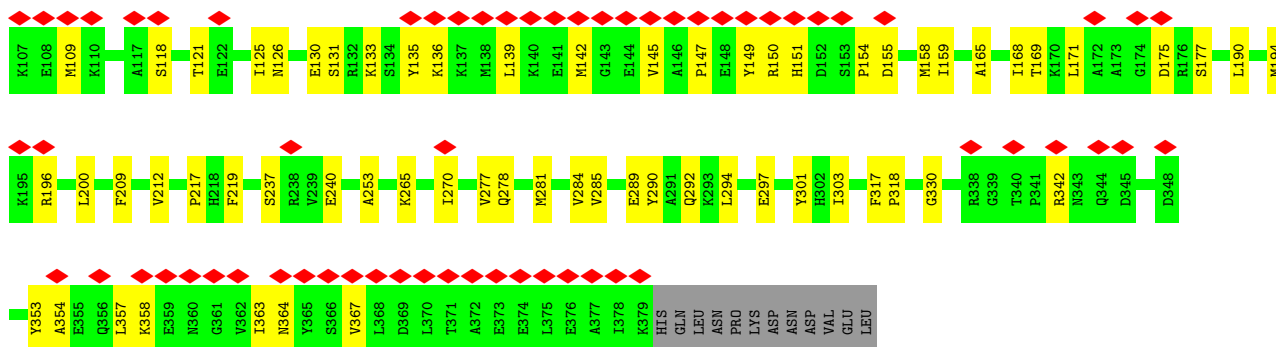


• Molecule 1: Nucleoprotein

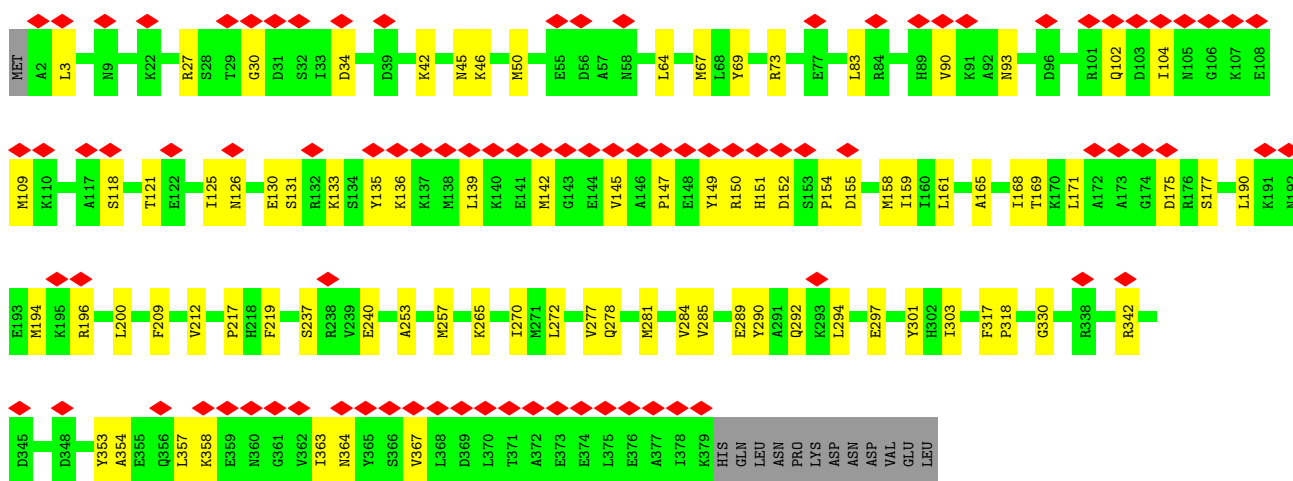
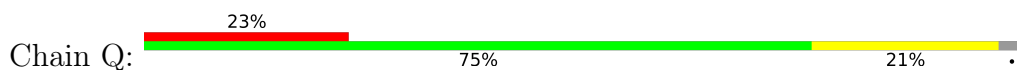


• Molecule 1: Nucleoprotein

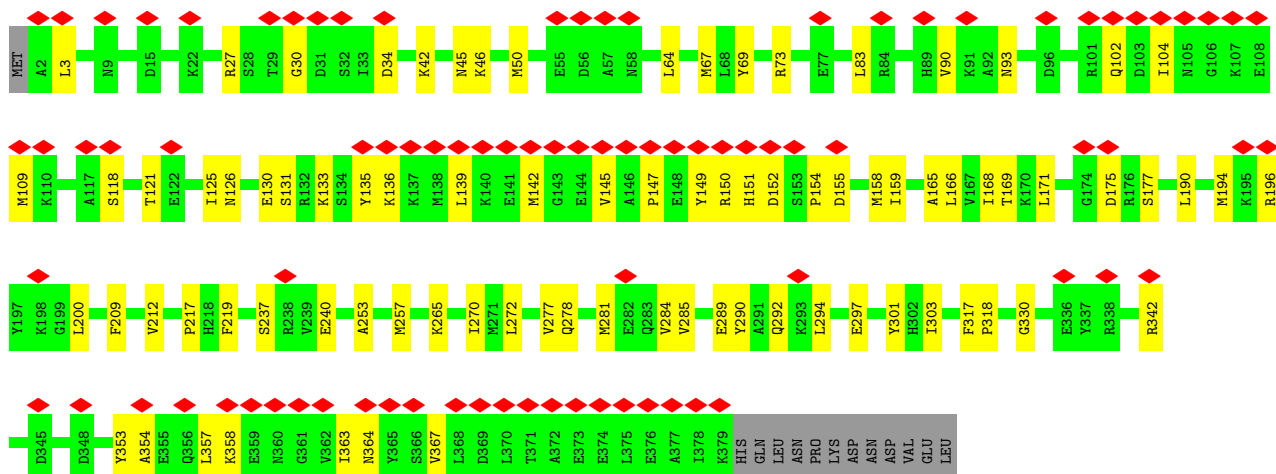
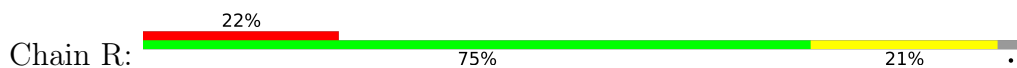




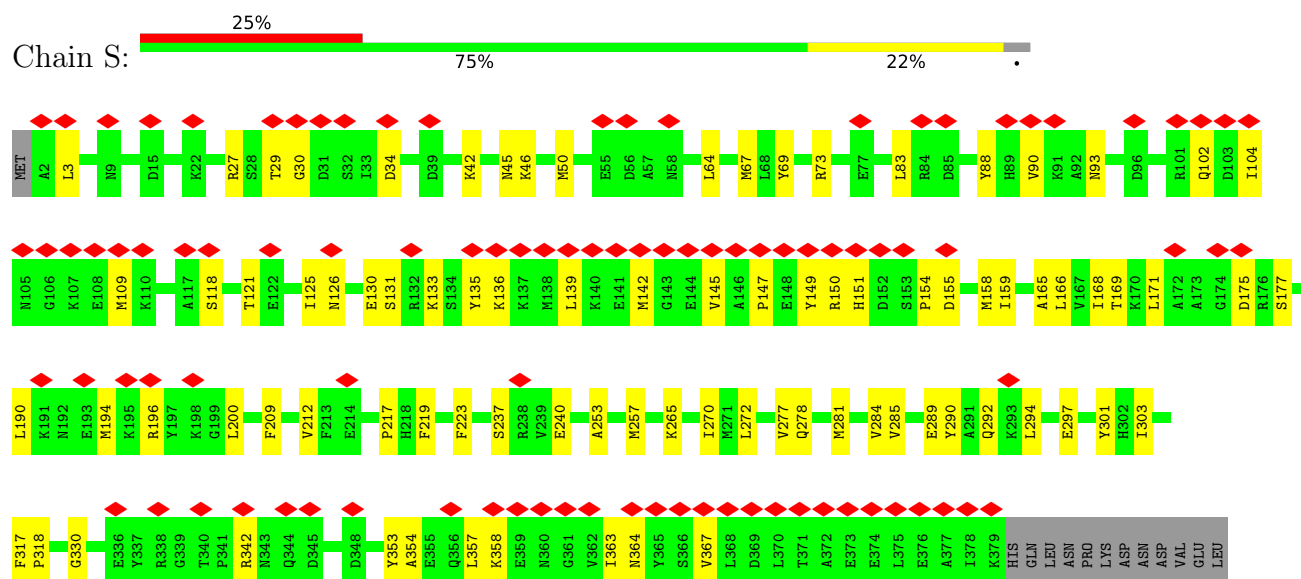
• Molecule 1: Nucleoprotein



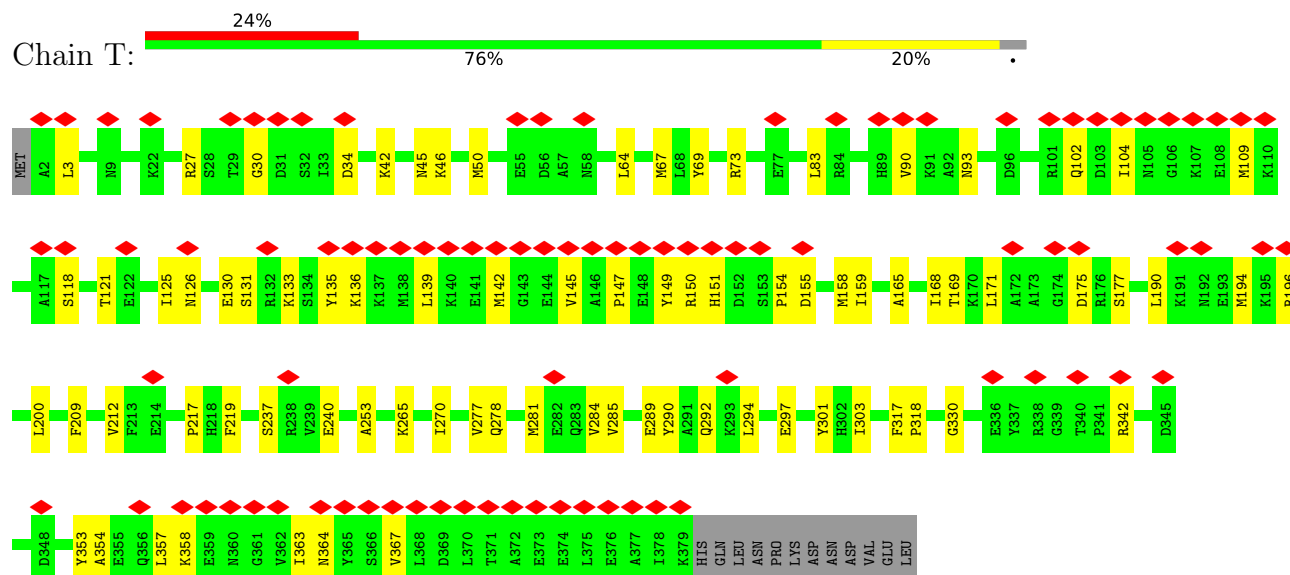
• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein



• Molecule 2: RNA (70-mer)



• Molecule 2: RNA (70-mer)



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, D10                              | Depositor |
| Number of particles used             | 47212                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS GLACIOS                             | Depositor |
| Voltage (kV)                         | 200                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 42                                      | Depositor |
| Minimum defocus (nm)                 | 700                                     | Depositor |
| Maximum defocus (nm)                 | 2400                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 3.215                                   | Depositor |
| Minimum map value                    | -1.883                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.058                                   | Depositor |
| Recommended contour level            | 0.7                                     | Depositor |
| Map size (Å)                         | 503.8, 503.8, 503.8                     | wwPDB     |
| Map dimensions                       | 440, 440, 440                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.145, 1.145, 1.145                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | A     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | B     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | C     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | D     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | E     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | F     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | G     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | H     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | I     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | J     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | K     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | L     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | M     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | N     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | O     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | P     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | Q     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | R     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | S     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 1   | T     | 0.23         | 0/3002      | 0.37        | 0/4044      |
| 2   | U     | 0.22         | 0/1530      | 0.23        | 0/2340      |
| 2   | e     | 0.22         | 0/1530      | 0.23        | 0/2340      |
| All | All   | 0.23         | 0/63100     | 0.36        | 0/85560     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2950  | 0        | 2985     | 63      | 0            |
| 1   | B     | 2950  | 0        | 2985     | 64      | 0            |
| 1   | C     | 2950  | 0        | 2985     | 62      | 0            |
| 1   | D     | 2950  | 0        | 2985     | 62      | 0            |
| 1   | E     | 2950  | 0        | 2985     | 64      | 0            |
| 1   | F     | 2950  | 0        | 2985     | 62      | 0            |
| 1   | G     | 2950  | 0        | 2985     | 63      | 0            |
| 1   | H     | 2950  | 0        | 2985     | 66      | 0            |
| 1   | I     | 2950  | 0        | 2985     | 63      | 0            |
| 1   | J     | 2950  | 0        | 2985     | 62      | 0            |
| 1   | K     | 2950  | 0        | 2985     | 62      | 0            |
| 1   | L     | 2950  | 0        | 2985     | 62      | 0            |
| 1   | M     | 2950  | 0        | 2985     | 61      | 0            |
| 1   | N     | 2950  | 0        | 2985     | 62      | 0            |
| 1   | O     | 2950  | 0        | 2985     | 64      | 0            |
| 1   | P     | 2950  | 0        | 2985     | 59      | 0            |
| 1   | Q     | 2950  | 0        | 2985     | 62      | 0            |
| 1   | R     | 2950  | 0        | 2985     | 62      | 0            |
| 1   | S     | 2950  | 0        | 2985     | 64      | 0            |
| 1   | T     | 2950  | 0        | 2985     | 60      | 0            |
| 2   | U     | 1400  | 0        | 780      | 18      | 0            |
| 2   | e     | 1400  | 0        | 780      | 18      | 0            |
| All | All   | 61800 | 0        | 61260    | 1151    | 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 9.

All (1151) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:194:MET:HG2 | 1:G:200:LEU:HD22 | 1.61                     | 0.83              |
| 1:Q:194:MET:HG2 | 1:Q:200:LEU:HD22 | 1.61                     | 0.83              |
| 1:A:194:MET:HG2 | 1:A:200:LEU:HD22 | 1.61                     | 0.83              |
| 1:H:194:MET:HG2 | 1:H:200:LEU:HD22 | 1.61                     | 0.83              |
| 1:K:194:MET:HG2 | 1:K:200:LEU:HD22 | 1.61                     | 0.83              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:R:194:MET:HG2 | 1:R:200:LEU:HD22 | 1.61                     | 0.83              |
| 1:T:194:MET:HG2 | 1:T:200:LEU:HD22 | 1.61                     | 0.83              |
| 1:J:194:MET:HG2 | 1:J:200:LEU:HD22 | 1.61                     | 0.83              |
| 1:B:194:MET:HG2 | 1:B:200:LEU:HD22 | 1.61                     | 0.83              |
| 1:L:194:MET:HG2 | 1:L:200:LEU:HD22 | 1.61                     | 0.83              |
| 1:E:194:MET:HG2 | 1:E:200:LEU:HD22 | 1.61                     | 0.83              |
| 1:I:194:MET:HG2 | 1:I:200:LEU:HD22 | 1.61                     | 0.83              |
| 1:M:194:MET:HG2 | 1:M:200:LEU:HD22 | 1.61                     | 0.83              |
| 1:O:194:MET:HG2 | 1:O:200:LEU:HD22 | 1.61                     | 0.83              |
| 1:C:194:MET:HG2 | 1:C:200:LEU:HD22 | 1.61                     | 0.82              |
| 1:P:194:MET:HG2 | 1:P:200:LEU:HD22 | 1.61                     | 0.82              |
| 1:S:194:MET:HG2 | 1:S:200:LEU:HD22 | 1.61                     | 0.82              |
| 1:F:194:MET:HG2 | 1:F:200:LEU:HD22 | 1.61                     | 0.82              |
| 1:D:194:MET:HG2 | 1:D:200:LEU:HD22 | 1.61                     | 0.82              |
| 1:N:194:MET:HG2 | 1:N:200:LEU:HD22 | 1.61                     | 0.82              |
| 1:C:64:LEU:HD11 | 1:C:118:SER:HB2  | 1.75                     | 0.69              |
| 1:M:64:LEU:HD11 | 1:M:118:SER:HB2  | 1.75                     | 0.69              |
| 1:D:64:LEU:HD11 | 1:D:118:SER:HB2  | 1.75                     | 0.68              |
| 1:N:64:LEU:HD11 | 1:N:118:SER:HB2  | 1.75                     | 0.68              |
| 1:J:64:LEU:HD11 | 1:J:118:SER:HB2  | 1.75                     | 0.68              |
| 1:T:64:LEU:HD11 | 1:T:118:SER:HB2  | 1.75                     | 0.68              |
| 1:I:64:LEU:HD11 | 1:I:118:SER:HB2  | 1.75                     | 0.68              |
| 1:L:64:LEU:HD11 | 1:L:118:SER:HB2  | 1.75                     | 0.68              |
| 1:Q:64:LEU:HD11 | 1:Q:118:SER:HB2  | 1.75                     | 0.68              |
| 1:R:64:LEU:HD11 | 1:R:118:SER:HB2  | 1.75                     | 0.68              |
| 1:S:64:LEU:HD11 | 1:S:118:SER:HB2  | 1.75                     | 0.68              |
| 1:G:64:LEU:HD11 | 1:G:118:SER:HB2  | 1.75                     | 0.68              |
| 1:H:64:LEU:HD11 | 1:H:118:SER:HB2  | 1.75                     | 0.68              |
| 1:P:64:LEU:HD11 | 1:P:118:SER:HB2  | 1.75                     | 0.68              |
| 1:A:64:LEU:HD11 | 1:A:118:SER:HB2  | 1.75                     | 0.67              |
| 1:B:64:LEU:HD11 | 1:B:118:SER:HB2  | 1.75                     | 0.67              |
| 1:F:64:LEU:HD11 | 1:F:118:SER:HB2  | 1.75                     | 0.67              |
| 1:K:64:LEU:HD11 | 1:K:118:SER:HB2  | 1.75                     | 0.67              |
| 1:A:67:MET:HE2  | 1:A:219:PHE:HB3  | 1.77                     | 0.67              |
| 1:K:67:MET:HE2  | 1:K:219:PHE:HB3  | 1.77                     | 0.67              |
| 1:L:67:MET:HE2  | 1:L:219:PHE:HB3  | 1.77                     | 0.67              |
| 1:B:67:MET:HE2  | 1:B:219:PHE:HB3  | 1.77                     | 0.67              |
| 1:J:67:MET:HE2  | 1:J:219:PHE:HB3  | 1.77                     | 0.67              |
| 1:O:64:LEU:HD11 | 1:O:118:SER:HB2  | 1.75                     | 0.67              |
| 1:T:67:MET:HE2  | 1:T:219:PHE:HB3  | 1.77                     | 0.67              |
| 1:E:64:LEU:HD11 | 1:E:118:SER:HB2  | 1.75                     | 0.66              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:F:67:MET:HE2 | 1:F:219:PHE:HB3 | 1.77                     | 0.66              |
| 1:J:285:VAL:O  | 1:J:289:GLU:HG3 | 1.95                     | 0.66              |
| 1:P:67:MET:HE2 | 1:P:219:PHE:HB3 | 1.77                     | 0.66              |
| 1:I:285:VAL:O  | 1:I:289:GLU:HG3 | 1.95                     | 0.66              |
| 1:M:67:MET:HE2 | 1:M:219:PHE:HB3 | 1.77                     | 0.66              |
| 1:T:285:VAL:O  | 1:T:289:GLU:HG3 | 1.95                     | 0.66              |
| 1:I:67:MET:HE2 | 1:I:219:PHE:HB3 | 1.77                     | 0.66              |
| 1:Q:67:MET:HE2 | 1:Q:219:PHE:HB3 | 1.77                     | 0.66              |
| 1:S:285:VAL:O  | 1:S:289:GLU:HG3 | 1.95                     | 0.66              |
| 1:C:67:MET:HE2 | 1:C:219:PHE:HB3 | 1.77                     | 0.66              |
| 1:A:285:VAL:O  | 1:A:289:GLU:HG3 | 1.95                     | 0.66              |
| 1:E:67:MET:HE2 | 1:E:219:PHE:HB3 | 1.77                     | 0.66              |
| 1:G:67:MET:HE2 | 1:G:219:PHE:HB3 | 1.77                     | 0.66              |
| 1:S:67:MET:HE2 | 1:S:219:PHE:HB3 | 1.77                     | 0.66              |
| 1:B:285:VAL:O  | 1:B:289:GLU:HG3 | 1.95                     | 0.66              |
| 1:O:67:MET:HE2 | 1:O:219:PHE:HB3 | 1.77                     | 0.66              |
| 1:K:285:VAL:O  | 1:K:289:GLU:HG3 | 1.95                     | 0.66              |
| 1:L:285:VAL:O  | 1:L:289:GLU:HG3 | 1.95                     | 0.66              |
| 1:N:285:VAL:O  | 1:N:289:GLU:HG3 | 1.95                     | 0.66              |
| 1:E:285:VAL:O  | 1:E:289:GLU:HG3 | 1.95                     | 0.66              |
| 1:O:285:VAL:O  | 1:O:289:GLU:HG3 | 1.95                     | 0.66              |
| 1:D:285:VAL:O  | 1:D:289:GLU:HG3 | 1.95                     | 0.66              |
| 1:P:285:VAL:O  | 1:P:289:GLU:HG3 | 1.95                     | 0.66              |
| 1:R:67:MET:HE2 | 1:R:219:PHE:HB3 | 1.77                     | 0.66              |
| 1:R:285:VAL:O  | 1:R:289:GLU:HG3 | 1.95                     | 0.66              |
| 1:F:285:VAL:O  | 1:F:289:GLU:HG3 | 1.95                     | 0.65              |
| 1:H:285:VAL:O  | 1:H:289:GLU:HG3 | 1.95                     | 0.65              |
| 1:M:285:VAL:O  | 1:M:289:GLU:HG3 | 1.95                     | 0.65              |
| 1:R:46:LYS:O   | 1:R:50:MET:HG3  | 1.96                     | 0.65              |
| 1:H:46:LYS:O   | 1:H:50:MET:HG3  | 1.96                     | 0.65              |
| 1:I:46:LYS:O   | 1:I:50:MET:HG3  | 1.96                     | 0.65              |
| 1:O:46:LYS:O   | 1:O:50:MET:HG3  | 1.96                     | 0.65              |
| 1:C:285:VAL:O  | 1:C:289:GLU:HG3 | 1.95                     | 0.65              |
| 1:D:67:MET:HE2 | 1:D:219:PHE:HB3 | 1.77                     | 0.65              |
| 1:E:46:LYS:O   | 1:E:50:MET:HG3  | 1.96                     | 0.65              |
| 1:F:46:LYS:O   | 1:F:50:MET:HG3  | 1.96                     | 0.65              |
| 1:H:67:MET:HE2 | 1:H:219:PHE:HB3 | 1.77                     | 0.65              |
| 1:S:46:LYS:O   | 1:S:50:MET:HG3  | 1.96                     | 0.65              |
| 1:P:46:LYS:O   | 1:P:50:MET:HG3  | 1.96                     | 0.65              |
| 1:G:285:VAL:O  | 1:G:289:GLU:HG3 | 1.95                     | 0.65              |
| 1:J:46:LYS:O   | 1:J:50:MET:HG3  | 1.96                     | 0.65              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:N:67:MET:HE2  | 1:N:219:PHE:HB3  | 1.77                     | 0.65              |
| 1:Q:285:VAL:O   | 1:Q:289:GLU:HG3  | 1.95                     | 0.65              |
| 1:T:46:LYS:O    | 1:T:50:MET:HG3   | 1.96                     | 0.65              |
| 1:C:253:ALA:HB3 | 1:C:303:ILE:HD11 | 1.79                     | 0.65              |
| 1:M:253:ALA:HB3 | 1:M:303:ILE:HD11 | 1.79                     | 0.65              |
| 1:K:46:LYS:O    | 1:K:50:MET:HG3   | 1.96                     | 0.65              |
| 1:A:46:LYS:O    | 1:A:50:MET:HG3   | 1.96                     | 0.65              |
| 1:J:253:ALA:HB3 | 1:J:303:ILE:HD11 | 1.79                     | 0.65              |
| 1:B:46:LYS:O    | 1:B:50:MET:HG3   | 1.96                     | 0.64              |
| 1:L:46:LYS:O    | 1:L:50:MET:HG3   | 1.96                     | 0.64              |
| 1:T:253:ALA:HB3 | 1:T:303:ILE:HD11 | 1.79                     | 0.64              |
| 1:D:46:LYS:O    | 1:D:50:MET:HG3   | 1.96                     | 0.64              |
| 1:I:253:ALA:HB3 | 1:I:303:ILE:HD11 | 1.79                     | 0.64              |
| 1:N:46:LYS:O    | 1:N:50:MET:HG3   | 1.96                     | 0.64              |
| 1:S:253:ALA:HB3 | 1:S:303:ILE:HD11 | 1.79                     | 0.64              |
| 1:D:253:ALA:HB3 | 1:D:303:ILE:HD11 | 1.79                     | 0.64              |
| 1:Q:46:LYS:O    | 1:Q:50:MET:HG3   | 1.96                     | 0.64              |
| 1:L:253:ALA:HB3 | 1:L:303:ILE:HD11 | 1.79                     | 0.64              |
| 1:N:253:ALA:HB3 | 1:N:303:ILE:HD11 | 1.79                     | 0.64              |
| 1:B:253:ALA:HB3 | 1:B:303:ILE:HD11 | 1.79                     | 0.64              |
| 1:G:46:LYS:O    | 1:G:50:MET:HG3   | 1.96                     | 0.64              |
| 1:A:253:ALA:HB3 | 1:A:303:ILE:HD11 | 1.79                     | 0.64              |
| 1:C:46:LYS:O    | 1:C:50:MET:HG3   | 1.96                     | 0.64              |
| 1:R:253:ALA:HB3 | 1:R:303:ILE:HD11 | 1.79                     | 0.64              |
| 1:H:253:ALA:HB3 | 1:H:303:ILE:HD11 | 1.79                     | 0.64              |
| 1:K:253:ALA:HB3 | 1:K:303:ILE:HD11 | 1.79                     | 0.63              |
| 1:M:46:LYS:O    | 1:M:50:MET:HG3   | 1.96                     | 0.63              |
| 1:Q:253:ALA:HB3 | 1:Q:303:ILE:HD11 | 1.79                     | 0.63              |
| 1:G:253:ALA:HB3 | 1:G:303:ILE:HD11 | 1.79                     | 0.63              |
| 1:P:253:ALA:HB3 | 1:P:303:ILE:HD11 | 1.79                     | 0.63              |
| 1:F:253:ALA:HB3 | 1:F:303:ILE:HD11 | 1.79                     | 0.63              |
| 1:E:253:ALA:HB3 | 1:E:303:ILE:HD11 | 1.79                     | 0.62              |
| 1:O:253:ALA:HB3 | 1:O:303:ILE:HD11 | 1.79                     | 0.62              |
| 1:B:102:GLN:NE2 | 1:B:125:ILE:HG21 | 2.15                     | 0.61              |
| 1:M:102:GLN:NE2 | 1:M:125:ILE:HG21 | 2.15                     | 0.61              |
| 1:C:102:GLN:NE2 | 1:C:125:ILE:HG21 | 2.15                     | 0.61              |
| 1:L:102:GLN:NE2 | 1:L:125:ILE:HG21 | 2.15                     | 0.61              |
| 1:D:102:GLN:NE2 | 1:D:125:ILE:HG21 | 2.15                     | 0.61              |
| 1:J:102:GLN:NE2 | 1:J:125:ILE:HG21 | 2.15                     | 0.61              |
| 1:T:102:GLN:NE2 | 1:T:125:ILE:HG21 | 2.15                     | 0.61              |
| 1:N:102:GLN:NE2 | 1:N:125:ILE:HG21 | 2.15                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:102:GLN:NE2  | 1:K:125:ILE:HG21 | 2.16                     | 0.61              |
| 1:A:102:GLN:NE2  | 1:A:125:ILE:HG21 | 2.16                     | 0.61              |
| 1:L:168:ILE:HD13 | 1:L:171:LEU:HD12 | 1.84                     | 0.60              |
| 1:A:168:ILE:HD13 | 1:A:171:LEU:HD12 | 1.84                     | 0.60              |
| 1:B:168:ILE:HD13 | 1:B:171:LEU:HD12 | 1.84                     | 0.60              |
| 1:K:168:ILE:HD13 | 1:K:171:LEU:HD12 | 1.84                     | 0.60              |
| 1:E:102:GLN:NE2  | 1:E:125:ILE:HG21 | 2.15                     | 0.60              |
| 1:H:102:GLN:NE2  | 1:H:125:ILE:HG21 | 2.15                     | 0.60              |
| 1:I:102:GLN:NE2  | 1:I:125:ILE:HG21 | 2.15                     | 0.60              |
| 1:J:168:ILE:HD13 | 1:J:171:LEU:HD12 | 1.84                     | 0.60              |
| 1:O:102:GLN:NE2  | 1:O:125:ILE:HG21 | 2.15                     | 0.60              |
| 1:R:102:GLN:NE2  | 1:R:125:ILE:HG21 | 2.15                     | 0.60              |
| 1:T:168:ILE:HD13 | 1:T:171:LEU:HD12 | 1.84                     | 0.60              |
| 1:F:168:ILE:HD13 | 1:F:171:LEU:HD12 | 1.84                     | 0.60              |
| 1:P:168:ILE:HD13 | 1:P:171:LEU:HD12 | 1.84                     | 0.60              |
| 1:Q:168:ILE:HD13 | 1:Q:171:LEU:HD12 | 1.84                     | 0.60              |
| 1:S:102:GLN:NE2  | 1:S:125:ILE:HG21 | 2.15                     | 0.60              |
| 1:G:168:ILE:HD13 | 1:G:171:LEU:HD12 | 1.84                     | 0.60              |
| 1:Q:102:GLN:NE2  | 1:Q:125:ILE:HG21 | 2.15                     | 0.60              |
| 1:F:102:GLN:NE2  | 1:F:125:ILE:HG21 | 2.16                     | 0.60              |
| 1:G:102:GLN:NE2  | 1:G:125:ILE:HG21 | 2.15                     | 0.60              |
| 1:M:168:ILE:HD13 | 1:M:171:LEU:HD12 | 1.83                     | 0.60              |
| 1:C:168:ILE:HD13 | 1:C:171:LEU:HD12 | 1.83                     | 0.60              |
| 1:E:168:ILE:HD13 | 1:E:171:LEU:HD12 | 1.84                     | 0.60              |
| 1:P:102:GLN:NE2  | 1:P:125:ILE:HG21 | 2.16                     | 0.60              |
| 1:I:168:ILE:HD13 | 1:I:171:LEU:HD12 | 1.84                     | 0.59              |
| 1:O:168:ILE:HD13 | 1:O:171:LEU:HD12 | 1.84                     | 0.59              |
| 1:S:168:ILE:HD13 | 1:S:171:LEU:HD12 | 1.84                     | 0.59              |
| 1:R:168:ILE:HD13 | 1:R:171:LEU:HD12 | 1.83                     | 0.59              |
| 1:H:168:ILE:HD13 | 1:H:171:LEU:HD12 | 1.83                     | 0.59              |
| 1:D:168:ILE:HD13 | 1:D:171:LEU:HD12 | 1.84                     | 0.59              |
| 1:N:168:ILE:HD13 | 1:N:171:LEU:HD12 | 1.84                     | 0.58              |
| 1:D:83:LEU:HD13  | 1:D:90:VAL:HG11  | 1.87                     | 0.57              |
| 1:N:83:LEU:HD13  | 1:N:90:VAL:HG11  | 1.87                     | 0.57              |
| 1:C:83:LEU:HD13  | 1:C:90:VAL:HG11  | 1.87                     | 0.57              |
| 1:M:83:LEU:HD13  | 1:M:90:VAL:HG11  | 1.87                     | 0.57              |
| 1:O:83:LEU:HD13  | 1:O:90:VAL:HG11  | 1.87                     | 0.56              |
| 1:B:83:LEU:HD13  | 1:B:90:VAL:HG11  | 1.87                     | 0.56              |
| 1:E:83:LEU:HD13  | 1:E:90:VAL:HG11  | 1.87                     | 0.56              |
| 1:F:27:ARG:NH1   | 1:G:240:GLU:OE1  | 2.39                     | 0.56              |
| 1:L:83:LEU:HD13  | 1:L:90:VAL:HG11  | 1.87                     | 0.56              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:P:27:ARG:NH1  | 1:Q:240:GLU:OE1 | 2.39                     | 0.56              |
| 1:E:27:ARG:NH1  | 1:F:240:GLU:OE1 | 2.39                     | 0.56              |
| 1:G:27:ARG:NH1  | 1:H:240:GLU:OE1 | 2.39                     | 0.56              |
| 1:O:27:ARG:NH1  | 1:P:240:GLU:OE1 | 2.39                     | 0.56              |
| 1:Q:27:ARG:NH1  | 1:R:240:GLU:OE1 | 2.39                     | 0.56              |
| 1:H:83:LEU:HD13 | 1:H:90:VAL:HG11 | 1.87                     | 0.56              |
| 1:R:83:LEU:HD13 | 1:R:90:VAL:HG11 | 1.87                     | 0.56              |
| 1:G:83:LEU:HD13 | 1:G:90:VAL:HG11 | 1.87                     | 0.56              |
| 1:I:83:LEU:HD13 | 1:I:90:VAL:HG11 | 1.87                     | 0.56              |
| 1:S:83:LEU:HD13 | 1:S:90:VAL:HG11 | 1.87                     | 0.56              |
| 1:D:27:ARG:NH1  | 1:E:240:GLU:OE1 | 2.39                     | 0.56              |
| 1:D:46:LYS:HG3  | 1:D:151:HIS:HD2 | 1.71                     | 0.56              |
| 1:N:27:ARG:NH1  | 1:O:240:GLU:OE1 | 2.39                     | 0.56              |
| 1:N:46:LYS:HG3  | 1:N:151:HIS:HD2 | 1.71                     | 0.56              |
| 1:P:83:LEU:HD13 | 1:P:90:VAL:HG11 | 1.87                     | 0.56              |
| 1:B:46:LYS:HG3  | 1:B:151:HIS:HD2 | 1.71                     | 0.55              |
| 1:H:27:ARG:NH1  | 1:I:240:GLU:OE1 | 2.39                     | 0.55              |
| 1:L:46:LYS:HG3  | 1:L:151:HIS:HD2 | 1.71                     | 0.55              |
| 1:Q:83:LEU:HD13 | 1:Q:90:VAL:HG11 | 1.87                     | 0.55              |
| 1:R:27:ARG:NH1  | 1:S:240:GLU:OE1 | 2.39                     | 0.55              |
| 1:F:83:LEU:HD13 | 1:F:90:VAL:HG11 | 1.87                     | 0.55              |
| 1:H:46:LYS:HG3  | 1:H:151:HIS:HD2 | 1.71                     | 0.55              |
| 1:R:46:LYS:HG3  | 1:R:151:HIS:HD2 | 1.71                     | 0.55              |
| 1:I:46:LYS:HG3  | 1:I:151:HIS:HD2 | 1.71                     | 0.55              |
| 1:E:126:ASN:O   | 1:E:130:GLU:HG2 | 2.07                     | 0.55              |
| 1:K:27:ARG:NH1  | 1:L:240:GLU:OE1 | 2.39                     | 0.55              |
| 1:O:126:ASN:O   | 1:O:130:GLU:HG2 | 2.07                     | 0.55              |
| 1:S:46:LYS:HG3  | 1:S:151:HIS:HD2 | 1.71                     | 0.55              |
| 1:B:126:ASN:O   | 1:B:130:GLU:HG2 | 2.07                     | 0.55              |
| 1:L:126:ASN:O   | 1:L:130:GLU:HG2 | 2.07                     | 0.55              |
| 1:T:83:LEU:HD13 | 1:T:90:VAL:HG11 | 1.87                     | 0.55              |
| 1:A:27:ARG:NH1  | 1:B:240:GLU:OE1 | 2.39                     | 0.55              |
| 1:J:83:LEU:HD13 | 1:J:90:VAL:HG11 | 1.87                     | 0.55              |
| 1:Q:149:TYR:HE1 | 1:Q:196:ARG:HA  | 1.72                     | 0.55              |
| 1:B:149:TYR:HE1 | 1:B:196:ARG:HA  | 1.72                     | 0.55              |
| 1:C:27:ARG:NH1  | 1:D:240:GLU:OE1 | 2.39                     | 0.55              |
| 1:G:149:TYR:HE1 | 1:G:196:ARG:HA  | 1.72                     | 0.55              |
| 1:I:126:ASN:O   | 1:I:130:GLU:HG2 | 2.07                     | 0.55              |
| 1:I:149:TYR:HE1 | 1:I:196:ARG:HA  | 1.72                     | 0.55              |
| 1:J:126:ASN:O   | 1:J:130:GLU:HG2 | 2.07                     | 0.55              |
| 1:K:46:LYS:HG3  | 1:K:151:HIS:HD2 | 1.71                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:L:149:TYR:HE1 | 1:L:196:ARG:HA   | 1.72                     | 0.55              |
| 1:M:27:ARG:NH1  | 1:N:240:GLU:OE1  | 2.39                     | 0.55              |
| 1:S:126:ASN:O   | 1:S:130:GLU:HG2  | 2.07                     | 0.55              |
| 1:S:149:TYR:HE1 | 1:S:196:ARG:HA   | 1.72                     | 0.55              |
| 1:A:46:LYS:HG3  | 1:A:151:HIS:HD2  | 1.71                     | 0.55              |
| 1:F:46:LYS:HG3  | 1:F:151:HIS:HD2  | 1.71                     | 0.55              |
| 1:I:281:MET:HA  | 1:I:284:VAL:HG22 | 1.89                     | 0.55              |
| 1:N:126:ASN:O   | 1:N:130:GLU:HG2  | 2.07                     | 0.55              |
| 1:S:281:MET:HA  | 1:S:284:VAL:HG22 | 1.89                     | 0.55              |
| 1:T:126:ASN:O   | 1:T:130:GLU:HG2  | 2.07                     | 0.55              |
| 1:A:83:LEU:HD13 | 1:A:90:VAL:HG11  | 1.87                     | 0.55              |
| 1:A:149:TYR:HE1 | 1:A:196:ARG:HA   | 1.72                     | 0.55              |
| 1:D:126:ASN:O   | 1:D:130:GLU:HG2  | 2.07                     | 0.55              |
| 1:H:149:TYR:HE1 | 1:H:196:ARG:HA   | 1.72                     | 0.55              |
| 1:K:149:TYR:HE1 | 1:K:196:ARG:HA   | 1.72                     | 0.55              |
| 1:P:46:LYS:HG3  | 1:P:151:HIS:HD2  | 1.71                     | 0.55              |
| 1:R:149:TYR:HE1 | 1:R:196:ARG:HA   | 1.72                     | 0.55              |
| 1:E:45:ASN:HD21 | 1:E:154:PRO:HA   | 1.72                     | 0.54              |
| 1:I:27:ARG:NH1  | 1:J:240:GLU:OE1  | 2.39                     | 0.54              |
| 1:N:45:ASN:HD21 | 1:N:154:PRO:HA   | 1.72                     | 0.54              |
| 1:O:45:ASN:HD21 | 1:O:154:PRO:HA   | 1.72                     | 0.54              |
| 1:S:27:ARG:NH1  | 1:T:240:GLU:OE1  | 2.39                     | 0.54              |
| 1:D:45:ASN:HD21 | 1:D:154:PRO:HA   | 1.72                     | 0.54              |
| 1:H:45:ASN:HD21 | 1:H:154:PRO:HA   | 1.72                     | 0.54              |
| 1:O:46:LYS:HG3  | 1:O:151:HIS:HD2  | 1.71                     | 0.54              |
| 1:P:149:TYR:HE1 | 1:P:196:ARG:HA   | 1.72                     | 0.54              |
| 1:R:281:MET:HA  | 1:R:284:VAL:HG22 | 1.89                     | 0.54              |
| 1:C:45:ASN:HD21 | 1:C:154:PRO:HA   | 1.72                     | 0.54              |
| 1:C:126:ASN:O   | 1:C:130:GLU:HG2  | 2.07                     | 0.54              |
| 1:C:149:TYR:HE1 | 1:C:196:ARG:HA   | 1.72                     | 0.54              |
| 1:F:126:ASN:O   | 1:F:130:GLU:HG2  | 2.07                     | 0.54              |
| 1:G:45:ASN:HD21 | 1:G:154:PRO:HA   | 1.72                     | 0.54              |
| 1:H:281:MET:HA  | 1:H:284:VAL:HG22 | 1.89                     | 0.54              |
| 1:K:83:LEU:HD13 | 1:K:90:VAL:HG11  | 1.87                     | 0.54              |
| 1:M:45:ASN:HD21 | 1:M:154:PRO:HA   | 1.72                     | 0.54              |
| 1:Q:45:ASN:HD21 | 1:Q:154:PRO:HA   | 1.72                     | 0.54              |
| 1:Q:297:GLU:OE2 | 1:Q:301:TYR:OH   | 2.20                     | 0.54              |
| 1:R:45:ASN:HD21 | 1:R:154:PRO:HA   | 1.72                     | 0.54              |
| 1:S:45:ASN:HD21 | 1:S:154:PRO:HA   | 1.72                     | 0.54              |
| 1:E:46:LYS:HG3  | 1:E:151:HIS:HD2  | 1.71                     | 0.54              |
| 1:F:149:TYR:HE1 | 1:F:196:ARG:HA   | 1.72                     | 0.54              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:I:45:ASN:HD21 | 1:I:154:PRO:HA   | 1.72                     | 0.54              |
| 1:P:126:ASN:O   | 1:P:130:GLU:HG2  | 2.07                     | 0.54              |
| 1:G:126:ASN:O   | 1:G:130:GLU:HG2  | 2.07                     | 0.54              |
| 1:M:126:ASN:O   | 1:M:130:GLU:HG2  | 2.07                     | 0.54              |
| 1:M:149:TYR:HE1 | 1:M:196:ARG:HA   | 1.72                     | 0.54              |
| 1:J:46:LYS:HG3  | 1:J:151:HIS:HD2  | 1.71                     | 0.54              |
| 1:M:46:LYS:HG3  | 1:M:151:HIS:HD2  | 1.71                     | 0.54              |
| 1:R:126:ASN:O   | 1:R:130:GLU:HG2  | 2.07                     | 0.54              |
| 1:T:46:LYS:HG3  | 1:T:151:HIS:HD2  | 1.71                     | 0.54              |
| 1:C:46:LYS:HG3  | 1:C:151:HIS:HD2  | 1.71                     | 0.54              |
| 1:E:142:MET:HE1 | 1:E:149:TYR:HD2  | 1.73                     | 0.54              |
| 1:G:297:GLU:OE2 | 1:G:301:TYR:OH   | 2.20                     | 0.54              |
| 1:H:126:ASN:O   | 1:H:130:GLU:HG2  | 2.07                     | 0.54              |
| 1:J:142:MET:HE1 | 1:J:149:TYR:HD2  | 1.73                     | 0.54              |
| 1:O:142:MET:HE1 | 1:O:149:TYR:HD2  | 1.73                     | 0.54              |
| 1:Q:126:ASN:O   | 1:Q:130:GLU:HG2  | 2.07                     | 0.54              |
| 1:T:142:MET:HE1 | 1:T:149:TYR:HD2  | 1.73                     | 0.54              |
| 1:T:149:TYR:HE1 | 1:T:196:ARG:HA   | 1.72                     | 0.54              |
| 1:J:149:TYR:HE1 | 1:J:196:ARG:HA   | 1.72                     | 0.54              |
| 1:J:281:MET:HA  | 1:J:284:VAL:HG22 | 1.89                     | 0.54              |
| 1:K:126:ASN:O   | 1:K:130:GLU:HG2  | 2.07                     | 0.54              |
| 1:L:27:ARG:NH1  | 1:M:240:GLU:OE1  | 2.39                     | 0.54              |
| 1:B:27:ARG:NH1  | 1:C:240:GLU:OE1  | 2.39                     | 0.54              |
| 1:L:297:GLU:OE2 | 1:L:301:TYR:OH   | 2.20                     | 0.54              |
| 1:A:126:ASN:O   | 1:A:130:GLU:HG2  | 2.07                     | 0.54              |
| 1:H:142:MET:HE1 | 1:H:149:TYR:HD2  | 1.73                     | 0.54              |
| 1:L:281:MET:HA  | 1:L:284:VAL:HG22 | 1.89                     | 0.54              |
| 1:N:142:MET:HE1 | 1:N:149:TYR:HD2  | 1.73                     | 0.54              |
| 1:Q:46:LYS:HG3  | 1:Q:151:HIS:HD2  | 1.71                     | 0.54              |
| 1:R:142:MET:HE1 | 1:R:149:TYR:HD2  | 1.73                     | 0.54              |
| 1:T:281:MET:HA  | 1:T:284:VAL:HG22 | 1.89                     | 0.54              |
| 1:B:45:ASN:HD21 | 1:B:154:PRO:HA   | 1.72                     | 0.53              |
| 1:B:281:MET:HA  | 1:B:284:VAL:HG22 | 1.89                     | 0.53              |
| 1:D:142:MET:HE1 | 1:D:149:TYR:HD2  | 1.73                     | 0.53              |
| 1:O:149:TYR:HE1 | 1:O:196:ARG:HA   | 1.72                     | 0.53              |
| 1:B:297:GLU:OE2 | 1:B:301:TYR:OH   | 2.20                     | 0.53              |
| 1:D:149:TYR:HE1 | 1:D:196:ARG:HA   | 1.72                     | 0.53              |
| 1:G:46:LYS:HG3  | 1:G:151:HIS:HD2  | 1.71                     | 0.53              |
| 1:K:281:MET:HA  | 1:K:284:VAL:HG22 | 1.89                     | 0.53              |
| 1:A:240:GLU:OE1 | 1:J:27:ARG:NH1   | 2.39                     | 0.53              |
| 1:B:142:MET:HE1 | 1:B:149:TYR:HD2  | 1.73                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:281:MET:HA   | 1:C:284:VAL:HG22 | 1.89                     | 0.53              |
| 1:L:45:ASN:HD21  | 1:L:154:PRO:HA   | 1.72                     | 0.53              |
| 1:L:142:MET:HE1  | 1:L:149:TYR:HD2  | 1.73                     | 0.53              |
| 1:M:281:MET:HA   | 1:M:284:VAL:HG22 | 1.89                     | 0.53              |
| 1:A:281:MET:HA   | 1:A:284:VAL:HG22 | 1.89                     | 0.53              |
| 1:D:139:LEU:HD13 | 1:D:145:VAL:HG13 | 1.91                     | 0.53              |
| 1:E:149:TYR:HE1  | 1:E:196:ARG:HA   | 1.72                     | 0.53              |
| 1:E:281:MET:HA   | 1:E:284:VAL:HG22 | 1.89                     | 0.53              |
| 1:F:281:MET:HA   | 1:F:284:VAL:HG22 | 1.89                     | 0.53              |
| 1:K:240:GLU:OE1  | 1:T:27:ARG:NH1   | 2.39                     | 0.53              |
| 1:N:139:LEU:HD13 | 1:N:145:VAL:HG13 | 1.91                     | 0.53              |
| 1:Q:142:MET:HE1  | 1:Q:149:TYR:HD2  | 1.73                     | 0.53              |
| 1:C:139:LEU:HD13 | 1:C:145:VAL:HG13 | 1.91                     | 0.53              |
| 1:E:139:LEU:HD13 | 1:E:145:VAL:HG13 | 1.91                     | 0.53              |
| 1:F:45:ASN:HD21  | 1:F:154:PRO:HA   | 1.72                     | 0.53              |
| 1:G:142:MET:HE1  | 1:G:149:TYR:HD2  | 1.73                     | 0.53              |
| 1:L:139:LEU:HD13 | 1:L:145:VAL:HG13 | 1.91                     | 0.53              |
| 1:M:139:LEU:HD13 | 1:M:145:VAL:HG13 | 1.91                     | 0.53              |
| 1:N:149:TYR:HE1  | 1:N:196:ARG:HA   | 1.72                     | 0.53              |
| 1:O:281:MET:HA   | 1:O:284:VAL:HG22 | 1.89                     | 0.53              |
| 1:P:281:MET:HA   | 1:P:284:VAL:HG22 | 1.89                     | 0.53              |
| 1:T:45:ASN:HD21  | 1:T:154:PRO:HA   | 1.72                     | 0.53              |
| 1:B:139:LEU:HD13 | 1:B:145:VAL:HG13 | 1.91                     | 0.53              |
| 1:D:281:MET:HA   | 1:D:284:VAL:HG22 | 1.89                     | 0.53              |
| 1:N:281:MET:HA   | 1:N:284:VAL:HG22 | 1.89                     | 0.53              |
| 1:O:139:LEU:HD13 | 1:O:145:VAL:HG13 | 1.91                     | 0.53              |
| 1:I:217:PRO:HG2  | 1:J:237:SER:HB3  | 1.91                     | 0.53              |
| 1:J:45:ASN:HD21  | 1:J:154:PRO:HA   | 1.72                     | 0.53              |
| 1:P:45:ASN:HD21  | 1:P:154:PRO:HA   | 1.72                     | 0.53              |
| 1:S:217:PRO:HG2  | 1:T:237:SER:HB3  | 1.91                     | 0.53              |
| 1:D:217:PRO:HG2  | 1:E:237:SER:HB3  | 1.91                     | 0.53              |
| 1:C:142:MET:HE1  | 1:C:149:TYR:HD2  | 1.73                     | 0.53              |
| 1:E:217:PRO:HG2  | 1:F:237:SER:HB3  | 1.91                     | 0.53              |
| 1:N:217:PRO:HG2  | 1:O:237:SER:HB3  | 1.91                     | 0.53              |
| 1:B:121:THR:O    | 1:B:125:ILE:HG12 | 2.09                     | 0.53              |
| 1:F:121:THR:O    | 1:F:125:ILE:HG12 | 2.09                     | 0.53              |
| 1:L:121:THR:O    | 1:L:125:ILE:HG12 | 2.09                     | 0.53              |
| 1:O:217:PRO:HG2  | 1:P:237:SER:HB3  | 1.91                     | 0.53              |
| 1:P:121:THR:O    | 1:P:125:ILE:HG12 | 2.09                     | 0.53              |
| 1:Q:281:MET:HA   | 1:Q:284:VAL:HG22 | 1.89                     | 0.53              |
| 1:G:281:MET:HA   | 1:G:284:VAL:HG22 | 1.89                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:142:MET:HE1  | 1:M:149:TYR:HD2  | 1.73                     | 0.52              |
| 1:D:121:THR:O    | 1:D:125:ILE:HG12 | 2.09                     | 0.52              |
| 1:F:165:ALA:O    | 1:F:169:THR:HG23 | 2.10                     | 0.52              |
| 1:I:158:MET:HE2  | 1:I:240:GLU:HG2  | 1.92                     | 0.52              |
| 1:I:165:ALA:O    | 1:I:169:THR:HG23 | 2.10                     | 0.52              |
| 1:J:158:MET:HE2  | 1:J:240:GLU:HG2  | 1.92                     | 0.52              |
| 1:K:139:LEU:HD13 | 1:K:145:VAL:HG13 | 1.91                     | 0.52              |
| 1:K:158:MET:HE2  | 1:K:240:GLU:HG2  | 1.92                     | 0.52              |
| 1:M:121:THR:O    | 1:M:125:ILE:HG12 | 2.09                     | 0.52              |
| 1:P:165:ALA:O    | 1:P:169:THR:HG23 | 2.10                     | 0.52              |
| 1:S:158:MET:HE2  | 1:S:240:GLU:HG2  | 1.92                     | 0.52              |
| 1:S:165:ALA:O    | 1:S:169:THR:HG23 | 2.10                     | 0.52              |
| 1:T:158:MET:HE2  | 1:T:240:GLU:HG2  | 1.92                     | 0.52              |
| 1:A:139:LEU:HD13 | 1:A:145:VAL:HG13 | 1.91                     | 0.52              |
| 1:A:158:MET:HE2  | 1:A:240:GLU:HG2  | 1.92                     | 0.52              |
| 1:C:121:THR:O    | 1:C:125:ILE:HG12 | 2.09                     | 0.52              |
| 1:E:121:THR:O    | 1:E:125:ILE:HG12 | 2.09                     | 0.52              |
| 1:F:217:PRO:HG2  | 1:G:237:SER:HB3  | 1.91                     | 0.52              |
| 1:H:158:MET:HE2  | 1:H:240:GLU:HG2  | 1.92                     | 0.52              |
| 1:I:142:MET:HE1  | 1:I:149:TYR:HD2  | 1.73                     | 0.52              |
| 1:J:165:ALA:O    | 1:J:169:THR:HG23 | 2.10                     | 0.52              |
| 1:M:217:PRO:HG2  | 1:N:237:SER:HB3  | 1.91                     | 0.52              |
| 1:N:121:THR:O    | 1:N:125:ILE:HG12 | 2.09                     | 0.52              |
| 1:P:217:PRO:HG2  | 1:Q:237:SER:HB3  | 1.91                     | 0.52              |
| 1:T:165:ALA:O    | 1:T:169:THR:HG23 | 2.10                     | 0.52              |
| 1:A:121:THR:O    | 1:A:125:ILE:HG12 | 2.09                     | 0.52              |
| 1:A:237:SER:HB3  | 1:J:217:PRO:HG2  | 1.91                     | 0.52              |
| 1:B:158:MET:HE2  | 1:B:240:GLU:HG2  | 1.92                     | 0.52              |
| 1:C:217:PRO:HG2  | 1:D:237:SER:HB3  | 1.91                     | 0.52              |
| 1:F:142:MET:HE1  | 1:F:149:TYR:HD2  | 1.73                     | 0.52              |
| 1:G:121:THR:O    | 1:G:125:ILE:HG12 | 2.09                     | 0.52              |
| 1:H:139:LEU:HD13 | 1:H:145:VAL:HG13 | 1.91                     | 0.52              |
| 1:I:139:LEU:HD13 | 1:I:145:VAL:HG13 | 1.91                     | 0.52              |
| 1:O:121:THR:O    | 1:O:125:ILE:HG12 | 2.09                     | 0.52              |
| 1:O:165:ALA:O    | 1:O:169:THR:HG23 | 2.10                     | 0.52              |
| 1:Q:121:THR:O    | 1:Q:125:ILE:HG12 | 2.09                     | 0.52              |
| 1:R:139:LEU:HD13 | 1:R:145:VAL:HG13 | 1.91                     | 0.52              |
| 1:R:158:MET:HE2  | 1:R:240:GLU:HG2  | 1.92                     | 0.52              |
| 1:S:139:LEU:HD13 | 1:S:145:VAL:HG13 | 1.91                     | 0.52              |
| 1:S:142:MET:HE1  | 1:S:149:TYR:HD2  | 1.73                     | 0.52              |
| 1:E:165:ALA:O    | 1:E:169:THR:HG23 | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:139:LEU:HD13 | 1:F:145:VAL:HG13 | 1.91                     | 0.52              |
| 1:K:121:THR:O    | 1:K:125:ILE:HG12 | 2.09                     | 0.52              |
| 1:K:237:SER:HB3  | 1:T:217:PRO:HG2  | 1.91                     | 0.52              |
| 1:L:158:MET:HE2  | 1:L:240:GLU:HG2  | 1.92                     | 0.52              |
| 1:R:217:PRO:HG2  | 1:S:237:SER:HB3  | 1.91                     | 0.52              |
| 1:C:158:MET:HE2  | 1:C:240:GLU:HG2  | 1.92                     | 0.52              |
| 1:H:217:PRO:HG2  | 1:I:237:SER:HB3  | 1.91                     | 0.52              |
| 1:P:142:MET:HE1  | 1:P:149:TYR:HD2  | 1.73                     | 0.52              |
| 1:G:158:MET:HE2  | 1:G:240:GLU:HG2  | 1.92                     | 0.52              |
| 1:G:165:ALA:O    | 1:G:169:THR:HG23 | 2.10                     | 0.52              |
| 1:M:158:MET:HE2  | 1:M:240:GLU:HG2  | 1.92                     | 0.52              |
| 1:P:139:LEU:HD13 | 1:P:145:VAL:HG13 | 1.91                     | 0.52              |
| 1:B:217:PRO:HG2  | 1:C:237:SER:HB3  | 1.91                     | 0.52              |
| 1:K:45:ASN:HD21  | 1:K:154:PRO:HA   | 1.72                     | 0.52              |
| 1:L:217:PRO:HG2  | 1:M:237:SER:HB3  | 1.91                     | 0.52              |
| 1:Q:158:MET:HE2  | 1:Q:240:GLU:HG2  | 1.92                     | 0.52              |
| 1:Q:165:ALA:O    | 1:Q:169:THR:HG23 | 2.10                     | 0.52              |
| 1:A:165:ALA:O    | 1:A:169:THR:HG23 | 2.10                     | 0.52              |
| 1:D:158:MET:HE2  | 1:D:240:GLU:HG2  | 1.92                     | 0.52              |
| 1:N:158:MET:HE2  | 1:N:240:GLU:HG2  | 1.92                     | 0.52              |
| 1:Q:139:LEU:HD13 | 1:Q:145:VAL:HG13 | 1.91                     | 0.52              |
| 1:A:45:ASN:HD21  | 1:A:154:PRO:HA   | 1.72                     | 0.52              |
| 1:G:139:LEU:HD13 | 1:G:145:VAL:HG13 | 1.91                     | 0.52              |
| 1:J:139:LEU:HD13 | 1:J:145:VAL:HG13 | 1.91                     | 0.52              |
| 1:K:142:MET:HE1  | 1:K:149:TYR:HD2  | 1.73                     | 0.52              |
| 1:R:165:ALA:O    | 1:R:169:THR:HG23 | 2.10                     | 0.52              |
| 1:G:217:PRO:HG2  | 1:H:237:SER:HB3  | 1.91                     | 0.51              |
| 1:H:165:ALA:O    | 1:H:169:THR:HG23 | 2.10                     | 0.51              |
| 1:I:278:GLN:HA   | 1:I:281:MET:HG2  | 1.92                     | 0.51              |
| 1:K:165:ALA:O    | 1:K:169:THR:HG23 | 2.10                     | 0.51              |
| 1:N:165:ALA:O    | 1:N:169:THR:HG23 | 2.10                     | 0.51              |
| 1:O:158:MET:HE2  | 1:O:240:GLU:HG2  | 1.92                     | 0.51              |
| 1:P:158:MET:HE2  | 1:P:240:GLU:HG2  | 1.92                     | 0.51              |
| 1:S:278:GLN:HA   | 1:S:281:MET:HG2  | 1.92                     | 0.51              |
| 1:A:142:MET:HE1  | 1:A:149:TYR:HD2  | 1.73                     | 0.51              |
| 1:E:158:MET:HE2  | 1:E:240:GLU:HG2  | 1.92                     | 0.51              |
| 1:F:158:MET:HE2  | 1:F:240:GLU:HG2  | 1.92                     | 0.51              |
| 1:J:121:THR:O    | 1:J:125:ILE:HG12 | 2.09                     | 0.51              |
| 1:O:297:GLU:OE2  | 1:O:301:TYR:OH   | 2.20                     | 0.51              |
| 1:Q:217:PRO:HG2  | 1:R:237:SER:HB3  | 1.91                     | 0.51              |
| 1:T:139:LEU:HD13 | 1:T:145:VAL:HG13 | 1.91                     | 0.51              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:165:ALA:O   | 1:D:169:THR:HG23 | 2.10                     | 0.51              |
| 1:F:278:GLN:HA  | 1:F:281:MET:HG2  | 1.92                     | 0.51              |
| 1:R:121:THR:O   | 1:R:125:ILE:HG12 | 2.09                     | 0.51              |
| 1:T:121:THR:O   | 1:T:125:ILE:HG12 | 2.09                     | 0.51              |
| 1:H:121:THR:O   | 1:H:125:ILE:HG12 | 2.09                     | 0.51              |
| 1:I:121:THR:O   | 1:I:125:ILE:HG12 | 2.09                     | 0.51              |
| 1:J:278:GLN:HA  | 1:J:281:MET:HG2  | 1.92                     | 0.51              |
| 1:P:278:GLN:HA  | 1:P:281:MET:HG2  | 1.92                     | 0.51              |
| 1:S:121:THR:O   | 1:S:125:ILE:HG12 | 2.09                     | 0.51              |
| 1:E:278:GLN:HA  | 1:E:281:MET:HG2  | 1.92                     | 0.51              |
| 1:O:278:GLN:HA  | 1:O:281:MET:HG2  | 1.92                     | 0.51              |
| 1:T:278:GLN:HA  | 1:T:281:MET:HG2  | 1.92                     | 0.51              |
| 1:D:278:GLN:HA  | 1:D:281:MET:HG2  | 1.92                     | 0.51              |
| 1:E:297:GLU:OE2 | 1:E:301:TYR:OH   | 2.20                     | 0.51              |
| 1:M:278:GLN:HA  | 1:M:281:MET:HG2  | 1.93                     | 0.51              |
| 1:N:278:GLN:HA  | 1:N:281:MET:HG2  | 1.92                     | 0.51              |
| 1:B:165:ALA:O   | 1:B:169:THR:HG23 | 2.10                     | 0.51              |
| 1:C:278:GLN:HA  | 1:C:281:MET:HG2  | 1.93                     | 0.51              |
| 1:L:278:GLN:HA  | 1:L:281:MET:HG2  | 1.92                     | 0.51              |
| 1:B:278:GLN:HA  | 1:B:281:MET:HG2  | 1.92                     | 0.51              |
| 1:B:318:PRO:HB3 | 1:B:342:ARG:HD2  | 1.93                     | 0.51              |
| 1:G:278:GLN:HA  | 1:G:281:MET:HG2  | 1.92                     | 0.51              |
| 1:K:217:PRO:HG2 | 1:L:237:SER:HB3  | 1.91                     | 0.51              |
| 1:L:318:PRO:HB3 | 1:L:342:ARG:HD2  | 1.93                     | 0.51              |
| 1:A:217:PRO:HG2 | 1:B:237:SER:HB3  | 1.91                     | 0.51              |
| 1:C:318:PRO:HB3 | 1:C:342:ARG:HD2  | 1.93                     | 0.51              |
| 1:F:318:PRO:HB3 | 1:F:342:ARG:HD2  | 1.93                     | 0.51              |
| 1:L:165:ALA:O   | 1:L:169:THR:HG23 | 2.10                     | 0.51              |
| 1:M:165:ALA:O   | 1:M:169:THR:HG23 | 2.10                     | 0.51              |
| 1:M:318:PRO:HB3 | 1:M:342:ARG:HD2  | 1.93                     | 0.51              |
| 1:P:318:PRO:HB3 | 1:P:342:ARG:HD2  | 1.93                     | 0.51              |
| 1:Q:278:GLN:HA  | 1:Q:281:MET:HG2  | 1.92                     | 0.51              |
| 1:A:318:PRO:HB3 | 1:A:342:ARG:HD2  | 1.93                     | 0.51              |
| 1:K:318:PRO:HB3 | 1:K:342:ARG:HD2  | 1.93                     | 0.51              |
| 1:R:278:GLN:HA  | 1:R:281:MET:HG2  | 1.93                     | 0.51              |
| 1:C:165:ALA:O   | 1:C:169:THR:HG23 | 2.10                     | 0.50              |
| 1:D:147:PRO:HA  | 1:D:150:ARG:HE   | 1.77                     | 0.50              |
| 1:G:318:PRO:HB3 | 1:G:342:ARG:HD2  | 1.93                     | 0.50              |
| 1:H:278:GLN:HA  | 1:H:281:MET:HG2  | 1.93                     | 0.50              |
| 1:N:147:PRO:HA  | 1:N:150:ARG:HE   | 1.77                     | 0.50              |
| 1:B:147:PRO:HA  | 1:B:150:ARG:HE   | 1.77                     | 0.50              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:3:LEU:HG    | 1:D:265:LYS:HG3 | 1.94                     | 0.50              |
| 1:L:147:PRO:HA  | 1:L:150:ARG:HE  | 1.77                     | 0.50              |
| 1:M:3:LEU:HG    | 1:N:265:LYS:HG3 | 1.94                     | 0.50              |
| 1:Q:318:PRO:HB3 | 1:Q:342:ARG:HD2 | 1.93                     | 0.50              |
| 1:B:3:LEU:HG    | 1:C:265:LYS:HG3 | 1.94                     | 0.50              |
| 1:E:277:VAL:O   | 1:E:281:MET:HG2 | 2.12                     | 0.50              |
| 1:I:277:VAL:O   | 1:I:281:MET:HG2 | 2.12                     | 0.50              |
| 1:N:318:PRO:HB3 | 1:N:342:ARG:HD2 | 1.93                     | 0.50              |
| 1:S:277:VAL:O   | 1:S:281:MET:HG2 | 2.12                     | 0.50              |
| 1:A:147:PRO:HA  | 1:A:150:ARG:HE  | 1.77                     | 0.50              |
| 1:D:318:PRO:HB3 | 1:D:342:ARG:HD2 | 1.93                     | 0.50              |
| 1:H:277:VAL:O   | 1:H:281:MET:HG2 | 2.12                     | 0.50              |
| 1:J:277:VAL:O   | 1:J:281:MET:HG2 | 2.12                     | 0.50              |
| 1:K:278:GLN:HA  | 1:K:281:MET:HG2 | 1.92                     | 0.50              |
| 1:L:3:LEU:HG    | 1:M:265:LYS:HG3 | 1.94                     | 0.50              |
| 1:O:277:VAL:O   | 1:O:281:MET:HG2 | 2.12                     | 0.50              |
| 1:T:277:VAL:O   | 1:T:281:MET:HG2 | 2.12                     | 0.50              |
| 1:A:278:GLN:HA  | 1:A:281:MET:HG2 | 1.92                     | 0.50              |
| 1:J:318:PRO:HB3 | 1:J:342:ARG:HD2 | 1.93                     | 0.50              |
| 1:O:147:PRO:HA  | 1:O:150:ARG:HE  | 1.77                     | 0.50              |
| 1:R:277:VAL:O   | 1:R:281:MET:HG2 | 2.12                     | 0.50              |
| 1:S:147:PRO:HA  | 1:S:150:ARG:HE  | 1.77                     | 0.50              |
| 1:S:318:PRO:HB3 | 1:S:342:ARG:HD2 | 1.93                     | 0.50              |
| 1:E:147:PRO:HA  | 1:E:150:ARG:HE  | 1.77                     | 0.50              |
| 1:I:147:PRO:HA  | 1:I:150:ARG:HE  | 1.77                     | 0.50              |
| 1:I:318:PRO:HB3 | 1:I:342:ARG:HD2 | 1.93                     | 0.50              |
| 1:K:147:PRO:HA  | 1:K:150:ARG:HE  | 1.77                     | 0.50              |
| 1:O:318:PRO:HB3 | 1:O:342:ARG:HD2 | 1.93                     | 0.50              |
| 1:T:318:PRO:HB3 | 1:T:342:ARG:HD2 | 1.93                     | 0.50              |
| 1:A:277:VAL:O   | 1:A:281:MET:HG2 | 2.12                     | 0.50              |
| 1:C:147:PRO:HA  | 1:C:150:ARG:HE  | 1.77                     | 0.50              |
| 1:E:318:PRO:HB3 | 1:E:342:ARG:HD2 | 1.93                     | 0.50              |
| 1:K:277:VAL:O   | 1:K:281:MET:HG2 | 2.12                     | 0.50              |
| 1:M:147:PRO:HA  | 1:M:150:ARG:HE  | 1.77                     | 0.50              |
| 1:R:297:GLU:OE2 | 1:R:301:TYR:OH  | 2.20                     | 0.50              |
| 1:C:277:VAL:O   | 1:C:281:MET:HG2 | 2.12                     | 0.49              |
| 1:F:3:LEU:HG    | 1:G:265:LYS:HG3 | 1.94                     | 0.49              |
| 1:H:147:PRO:HA  | 1:H:150:ARG:HE  | 1.77                     | 0.49              |
| 1:K:297:GLU:OE2 | 1:K:301:TYR:OH  | 2.20                     | 0.49              |
| 1:Q:277:VAL:O   | 1:Q:281:MET:HG2 | 2.12                     | 0.49              |
| 1:G:277:VAL:O   | 1:G:281:MET:HG2 | 2.12                     | 0.49              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:M:277:VAL:O    | 1:M:281:MET:HG2 | 2.12                     | 0.49              |
| 1:N:3:LEU:HG     | 1:O:265:LYS:HG3 | 1.94                     | 0.49              |
| 1:P:3:LEU:HG     | 1:Q:265:LYS:HG3 | 1.94                     | 0.49              |
| 1:R:147:PRO:HA   | 1:R:150:ARG:HE  | 1.77                     | 0.49              |
| 1:A:3:LEU:HG     | 1:B:265:LYS:HG3 | 1.94                     | 0.49              |
| 1:D:270:ILE:HG12 | 1:D:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:F:147:PRO:HA   | 1:F:150:ARG:HE  | 1.77                     | 0.49              |
| 1:L:277:VAL:O    | 1:L:281:MET:HG2 | 2.12                     | 0.49              |
| 1:N:270:ILE:HG12 | 1:N:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:O:270:ILE:HG12 | 1:O:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:R:318:PRO:HB3  | 1:R:342:ARG:HD2 | 1.93                     | 0.49              |
| 1:B:277:VAL:O    | 1:B:281:MET:HG2 | 2.12                     | 0.49              |
| 1:C:270:ILE:HG12 | 1:C:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:D:3:LEU:HG     | 1:E:265:LYS:HG3 | 1.94                     | 0.49              |
| 1:E:270:ILE:HG12 | 1:E:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:G:3:LEU:HG     | 1:H:265:LYS:HG3 | 1.94                     | 0.49              |
| 1:P:147:PRO:HA   | 1:P:150:ARG:HE  | 1.77                     | 0.49              |
| 1:B:270:ILE:HG12 | 1:B:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:F:277:VAL:O    | 1:F:281:MET:HG2 | 2.12                     | 0.49              |
| 1:H:297:GLU:OE2  | 1:H:301:TYR:OH  | 2.20                     | 0.49              |
| 1:H:318:PRO:HB3  | 1:H:342:ARG:HD2 | 1.93                     | 0.49              |
| 1:K:3:LEU:HG     | 1:L:265:LYS:HG3 | 1.94                     | 0.49              |
| 1:M:270:ILE:HG12 | 1:M:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:N:277:VAL:O    | 1:N:281:MET:HG2 | 2.12                     | 0.49              |
| 1:Q:3:LEU:HG     | 1:R:265:LYS:HG3 | 1.94                     | 0.49              |
| 1:R:3:LEU:HG     | 1:S:265:LYS:HG3 | 1.94                     | 0.49              |
| 1:A:297:GLU:OE2  | 1:A:301:TYR:OH  | 2.20                     | 0.49              |
| 1:E:3:LEU:HG     | 1:F:265:LYS:HG3 | 1.94                     | 0.49              |
| 1:F:270:ILE:HG12 | 1:F:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:G:147:PRO:HA   | 1:G:150:ARG:HE  | 1.77                     | 0.49              |
| 1:H:3:LEU:HG     | 1:I:265:LYS:HG3 | 1.94                     | 0.49              |
| 1:L:270:ILE:HG12 | 1:L:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:P:270:ILE:HG12 | 1:P:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:D:277:VAL:O    | 1:D:281:MET:HG2 | 2.12                     | 0.49              |
| 1:P:277:VAL:O    | 1:P:281:MET:HG2 | 2.12                     | 0.49              |
| 1:Q:147:PRO:HA   | 1:Q:150:ARG:HE  | 1.77                     | 0.49              |
| 1:T:147:PRO:HA   | 1:T:150:ARG:HE  | 1.77                     | 0.49              |
| 1:G:133:LYS:HA   | 1:G:136:LYS:HE3 | 1.95                     | 0.49              |
| 1:J:270:ILE:HG12 | 1:J:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:O:3:LEU:HG     | 1:P:265:LYS:HG3 | 1.94                     | 0.49              |
| 1:Q:133:LYS:HA   | 1:Q:136:LYS:HE3 | 1.95                     | 0.49              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:S:3:LEU:HG     | 1:T:265:LYS:HG3 | 1.94                     | 0.49              |
| 1:T:270:ILE:HG12 | 1:T:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:A:270:ILE:HG12 | 1:A:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:B:133:LYS:HA   | 1:B:136:LYS:HE3 | 1.95                     | 0.49              |
| 1:I:3:LEU:HG     | 1:J:265:LYS:HG3 | 1.94                     | 0.49              |
| 1:J:147:PRO:HA   | 1:J:150:ARG:HE  | 1.77                     | 0.49              |
| 1:L:133:LYS:HA   | 1:L:136:LYS:HE3 | 1.95                     | 0.49              |
| 1:Q:270:ILE:HG12 | 1:Q:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:C:133:LYS:HA   | 1:C:136:LYS:HE3 | 1.95                     | 0.49              |
| 1:G:270:ILE:HG12 | 1:G:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:K:265:LYS:HG3  | 1:T:3:LEU:HG    | 1.94                     | 0.49              |
| 1:K:270:ILE:HG12 | 1:K:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:M:133:LYS:HA   | 1:M:136:LYS:HE3 | 1.95                     | 0.49              |
| 1:P:133:LYS:HA   | 1:P:136:LYS:HE3 | 1.95                     | 0.49              |
| 1:S:270:ILE:HG12 | 1:S:353:TYR:CZ  | 2.48                     | 0.49              |
| 1:T:133:LYS:HA   | 1:T:136:LYS:HE3 | 1.95                     | 0.49              |
| 1:A:133:LYS:HA   | 1:A:136:LYS:HE3 | 1.95                     | 0.48              |
| 1:C:30:GLY:HA2   | 1:D:42:LYS:NZ   | 2.29                     | 0.48              |
| 1:F:133:LYS:HA   | 1:F:136:LYS:HE3 | 1.95                     | 0.48              |
| 1:I:270:ILE:HG12 | 1:I:353:TYR:CZ  | 2.48                     | 0.48              |
| 1:J:133:LYS:HA   | 1:J:136:LYS:HE3 | 1.95                     | 0.48              |
| 1:K:133:LYS:HA   | 1:K:136:LYS:HE3 | 1.95                     | 0.48              |
| 1:A:265:LYS:HG3  | 1:J:3:LEU:HG    | 1.94                     | 0.48              |
| 1:D:133:LYS:HA   | 1:D:136:LYS:HE3 | 1.95                     | 0.48              |
| 1:E:133:LYS:HA   | 1:E:136:LYS:HE3 | 1.95                     | 0.48              |
| 1:I:133:LYS:HA   | 1:I:136:LYS:HE3 | 1.95                     | 0.48              |
| 1:M:30:GLY:HA2   | 1:N:42:LYS:NZ   | 2.29                     | 0.48              |
| 1:R:133:LYS:HA   | 1:R:136:LYS:HE3 | 1.95                     | 0.48              |
| 1:S:133:LYS:HA   | 1:S:136:LYS:HE3 | 1.95                     | 0.48              |
| 1:E:30:GLY:HA2   | 1:F:42:LYS:NZ   | 2.29                     | 0.48              |
| 1:H:133:LYS:HA   | 1:H:136:LYS:HE3 | 1.95                     | 0.48              |
| 1:N:133:LYS:HA   | 1:N:136:LYS:HE3 | 1.95                     | 0.48              |
| 1:O:133:LYS:HA   | 1:O:136:LYS:HE3 | 1.95                     | 0.48              |
| 1:D:30:GLY:HA2   | 1:E:42:LYS:NZ   | 2.29                     | 0.48              |
| 1:F:30:GLY:HA2   | 1:G:42:LYS:NZ   | 2.29                     | 0.48              |
| 1:O:30:GLY:HA2   | 1:P:42:LYS:NZ   | 2.29                     | 0.48              |
| 1:P:30:GLY:HA2   | 1:Q:42:LYS:NZ   | 2.29                     | 0.48              |
| 1:R:270:ILE:HG12 | 1:R:353:TYR:CZ  | 2.48                     | 0.48              |
| 1:D:149:TYR:CE1  | 1:D:196:ARG:HG3 | 2.49                     | 0.48              |
| 1:H:270:ILE:HG12 | 1:H:353:TYR:CZ  | 2.48                     | 0.48              |
| 1:N:30:GLY:HA2   | 1:O:42:LYS:NZ   | 2.29                     | 0.48              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:149:TYR:CE1 | 1:E:196:ARG:HG3  | 2.49                     | 0.48              |
| 1:N:149:TYR:CE1 | 1:N:196:ARG:HG3  | 2.49                     | 0.48              |
| 1:O:149:TYR:CE1 | 1:O:196:ARG:HG3  | 2.49                     | 0.48              |
| 1:Q:30:GLY:HA2  | 1:R:42:LYS:NZ    | 2.28                     | 0.48              |
| 1:A:42:LYS:HZ1  | 1:J:30:GLY:HA2   | 1.79                     | 0.48              |
| 1:B:30:GLY:HA2  | 1:C:42:LYS:NZ    | 2.28                     | 0.48              |
| 1:B:149:TYR:CE1 | 1:B:196:ARG:HG3  | 2.49                     | 0.48              |
| 1:C:149:TYR:CE1 | 1:C:196:ARG:HG3  | 2.49                     | 0.48              |
| 1:G:30:GLY:HA2  | 1:H:42:LYS:NZ    | 2.28                     | 0.48              |
| 1:I:209:PHE:HA  | 1:I:212:VAL:HG12 | 1.96                     | 0.48              |
| 1:L:149:TYR:CE1 | 1:L:196:ARG:HG3  | 2.49                     | 0.48              |
| 1:J:209:PHE:HA  | 1:J:212:VAL:HG12 | 1.96                     | 0.48              |
| 1:M:149:TYR:CE1 | 1:M:196:ARG:HG3  | 2.49                     | 0.48              |
| 1:P:149:TYR:CE1 | 1:P:196:ARG:HG3  | 2.49                     | 0.48              |
| 1:S:209:PHE:HA  | 1:S:212:VAL:HG12 | 1.96                     | 0.48              |
| 1:T:209:PHE:HA  | 1:T:212:VAL:HG12 | 1.96                     | 0.48              |
| 1:F:149:TYR:CE1 | 1:F:196:ARG:HG3  | 2.49                     | 0.48              |
| 1:L:30:GLY:HA2  | 1:M:42:LYS:NZ    | 2.28                     | 0.48              |
| 1:H:209:PHE:HA  | 1:H:212:VAL:HG12 | 1.96                     | 0.47              |
| 1:R:209:PHE:HA  | 1:R:212:VAL:HG12 | 1.96                     | 0.47              |
| 1:A:209:PHE:HA  | 1:A:212:VAL:HG12 | 1.96                     | 0.47              |
| 1:D:69:TYR:CE2  | 1:D:73:ARG:HD2   | 2.50                     | 0.47              |
| 1:K:209:PHE:HA  | 1:K:212:VAL:HG12 | 1.96                     | 0.47              |
| 1:A:42:LYS:NZ   | 1:J:30:GLY:HA2   | 2.29                     | 0.47              |
| 1:C:69:TYR:CE2  | 1:C:73:ARG:HD2   | 2.50                     | 0.47              |
| 1:E:69:TYR:CE2  | 1:E:73:ARG:HD2   | 2.49                     | 0.47              |
| 1:K:42:LYS:NZ   | 1:T:30:GLY:HA2   | 2.29                     | 0.47              |
| 1:K:149:TYR:CE1 | 1:K:196:ARG:HG3  | 2.49                     | 0.47              |
| 1:M:69:TYR:CE2  | 1:M:73:ARG:HD2   | 2.50                     | 0.47              |
| 1:N:69:TYR:CE2  | 1:N:73:ARG:HD2   | 2.50                     | 0.47              |
| 1:O:69:TYR:CE2  | 1:O:73:ARG:HD2   | 2.49                     | 0.47              |
| 1:Q:149:TYR:CE1 | 1:Q:196:ARG:HG3  | 2.49                     | 0.47              |
| 1:R:30:GLY:HA2  | 1:S:42:LYS:NZ    | 2.29                     | 0.47              |
| 1:A:149:TYR:CE1 | 1:A:196:ARG:HG3  | 2.49                     | 0.47              |
| 1:B:69:TYR:CE2  | 1:B:73:ARG:HD2   | 2.49                     | 0.47              |
| 1:C:209:PHE:HA  | 1:C:212:VAL:HG12 | 1.96                     | 0.47              |
| 1:G:149:TYR:CE1 | 1:G:196:ARG:HG3  | 2.49                     | 0.47              |
| 1:H:30:GLY:HA2  | 1:I:42:LYS:NZ    | 2.29                     | 0.47              |
| 1:L:69:TYR:CE2  | 1:L:73:ARG:HD2   | 2.49                     | 0.47              |
| 1:M:209:PHE:HA  | 1:M:212:VAL:HG12 | 1.96                     | 0.47              |
| 1:K:30:GLY:HA2  | 1:L:42:LYS:NZ    | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:30:GLY:HA2   | 1:B:42:LYS:NZ    | 2.29                     | 0.47              |
| 1:G:209:PHE:HA   | 1:G:212:VAL:HG12 | 1.96                     | 0.47              |
| 1:H:149:TYR:CE1  | 1:H:196:ARG:HG3  | 2.49                     | 0.47              |
| 1:I:149:TYR:CE1  | 1:I:196:ARG:HG3  | 2.49                     | 0.47              |
| 1:K:69:TYR:CE2   | 1:K:73:ARG:HD2   | 2.49                     | 0.47              |
| 1:R:149:TYR:CE1  | 1:R:196:ARG:HG3  | 2.49                     | 0.47              |
| 1:S:149:TYR:CE1  | 1:S:196:ARG:HG3  | 2.49                     | 0.47              |
| 1:T:149:TYR:CE1  | 1:T:196:ARG:HG3  | 2.49                     | 0.47              |
| 1:A:69:TYR:CE2   | 1:A:73:ARG:HD2   | 2.49                     | 0.47              |
| 1:H:69:TYR:CE2   | 1:H:73:ARG:HD2   | 2.50                     | 0.47              |
| 1:I:30:GLY:HA2   | 1:J:42:LYS:NZ    | 2.29                     | 0.47              |
| 1:J:149:TYR:CE1  | 1:J:196:ARG:HG3  | 2.49                     | 0.47              |
| 1:Q:209:PHE:HA   | 1:Q:212:VAL:HG12 | 1.96                     | 0.47              |
| 1:R:69:TYR:CE2   | 1:R:73:ARG:HD2   | 2.50                     | 0.47              |
| 1:S:30:GLY:HA2   | 1:T:42:LYS:NZ    | 2.29                     | 0.47              |
| 1:D:209:PHE:HA   | 1:D:212:VAL:HG12 | 1.96                     | 0.47              |
| 1:F:69:TYR:CE2   | 1:F:73:ARG:HD2   | 2.49                     | 0.47              |
| 1:F:209:PHE:HA   | 1:F:212:VAL:HG12 | 1.96                     | 0.47              |
| 1:M:297:GLU:OE2  | 1:M:301:TYR:OH   | 2.20                     | 0.47              |
| 1:P:209:PHE:HA   | 1:P:212:VAL:HG12 | 1.96                     | 0.47              |
| 1:B:209:PHE:HA   | 1:B:212:VAL:HG12 | 1.96                     | 0.47              |
| 1:C:270:ILE:HG22 | 1:D:363:ILE:HD13 | 1.97                     | 0.47              |
| 1:G:69:TYR:CE2   | 1:G:73:ARG:HD2   | 2.49                     | 0.47              |
| 1:H:270:ILE:HG22 | 1:I:363:ILE:HD13 | 1.97                     | 0.47              |
| 1:L:209:PHE:HA   | 1:L:212:VAL:HG12 | 1.96                     | 0.47              |
| 1:M:270:ILE:HG22 | 1:N:363:ILE:HD13 | 1.97                     | 0.47              |
| 1:O:209:PHE:HA   | 1:O:212:VAL:HG12 | 1.96                     | 0.47              |
| 1:P:69:TYR:CE2   | 1:P:73:ARG:HD2   | 2.49                     | 0.47              |
| 1:R:270:ILE:HG22 | 1:S:363:ILE:HD13 | 1.97                     | 0.47              |
| 1:T:69:TYR:CE2   | 1:T:73:ARG:HD2   | 2.49                     | 0.47              |
| 1:I:69:TYR:CE2   | 1:I:73:ARG:HD2   | 2.50                     | 0.46              |
| 1:N:209:PHE:HA   | 1:N:212:VAL:HG12 | 1.96                     | 0.46              |
| 1:Q:69:TYR:CE2   | 1:Q:73:ARG:HD2   | 2.49                     | 0.46              |
| 1:S:69:TYR:CE2   | 1:S:73:ARG:HD2   | 2.50                     | 0.46              |
| 1:D:142:MET:HE1  | 1:D:149:TYR:CD2  | 2.51                     | 0.46              |
| 1:D:270:ILE:HG22 | 1:E:363:ILE:HD13 | 1.98                     | 0.46              |
| 1:E:209:PHE:HA   | 1:E:212:VAL:HG12 | 1.96                     | 0.46              |
| 1:I:257:MET:HE3  | 1:I:257:MET:HB3  | 1.83                     | 0.46              |
| 1:I:270:ILE:HG22 | 1:J:363:ILE:HD13 | 1.98                     | 0.46              |
| 1:J:69:TYR:CE2   | 1:J:73:ARG:HD2   | 2.49                     | 0.46              |
| 1:N:142:MET:HE1  | 1:N:149:TYR:CD2  | 2.51                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:270:ILE:HG22 | 1:O:363:ILE:HD13 | 1.98                     | 0.46              |
| 1:N:297:GLU:OE2  | 1:N:301:TYR:OH   | 2.20                     | 0.46              |
| 1:S:270:ILE:HG22 | 1:T:363:ILE:HD13 | 1.98                     | 0.46              |
| 1:A:363:ILE:HD13 | 1:J:270:ILE:HG22 | 1.97                     | 0.46              |
| 1:B:270:ILE:HG22 | 1:C:363:ILE:HD13 | 1.97                     | 0.46              |
| 1:G:270:ILE:HG22 | 1:H:363:ILE:HD13 | 1.97                     | 0.46              |
| 1:K:42:LYS:HZ1   | 1:T:30:GLY:HA2   | 1.80                     | 0.46              |
| 1:K:363:ILE:HD13 | 1:T:270:ILE:HG22 | 1.97                     | 0.46              |
| 1:O:270:ILE:HG22 | 1:P:363:ILE:HD13 | 1.97                     | 0.46              |
| 1:Q:270:ILE:HG22 | 1:R:363:ILE:HD13 | 1.97                     | 0.46              |
| 1:B:142:MET:HE1  | 1:B:149:TYR:CD2  | 2.51                     | 0.46              |
| 1:C:297:GLU:OE2  | 1:C:301:TYR:OH   | 2.20                     | 0.46              |
| 1:E:270:ILE:HG22 | 1:F:363:ILE:HD13 | 1.97                     | 0.46              |
| 1:K:257:MET:HE3  | 1:K:257:MET:HB3  | 1.83                     | 0.46              |
| 1:K:270:ILE:HG22 | 1:L:363:ILE:HD13 | 1.97                     | 0.46              |
| 1:L:142:MET:HE1  | 1:L:149:TYR:CD2  | 2.51                     | 0.46              |
| 1:L:270:ILE:HG22 | 1:M:363:ILE:HD13 | 1.97                     | 0.46              |
| 1:A:270:ILE:HG22 | 1:B:363:ILE:HD13 | 1.97                     | 0.46              |
| 1:P:270:ILE:HG22 | 1:Q:363:ILE:HD13 | 1.97                     | 0.46              |
| 1:F:142:MET:HE1  | 1:F:149:TYR:CD2  | 2.51                     | 0.46              |
| 1:P:142:MET:HE1  | 1:P:149:TYR:CD2  | 2.51                     | 0.46              |
| 1:S:257:MET:HE3  | 1:S:257:MET:HB3  | 1.83                     | 0.46              |
| 1:D:297:GLU:OE2  | 1:D:301:TYR:OH   | 2.20                     | 0.46              |
| 1:F:270:ILE:HG22 | 1:G:363:ILE:HD13 | 1.97                     | 0.46              |
| 1:L:30:GLY:HA2   | 1:M:42:LYS:HZ1   | 1.80                     | 0.46              |
| 1:D:30:GLY:HA2   | 1:E:42:LYS:HZ1   | 1.80                     | 0.45              |
| 1:O:272:LEU:O    | 1:O:278:GLN:NE2  | 2.46                     | 0.45              |
| 1:P:297:GLU:OE2  | 1:P:301:TYR:OH   | 2.20                     | 0.45              |
| 1:R:142:MET:HE1  | 1:R:149:TYR:CD2  | 2.51                     | 0.45              |
| 1:B:175:ASP:OD1  | 1:B:177:SER:HB2  | 2.17                     | 0.45              |
| 1:H:142:MET:HE1  | 1:H:149:TYR:CD2  | 2.51                     | 0.45              |
| 1:J:142:MET:HE1  | 1:J:149:TYR:CD2  | 2.51                     | 0.45              |
| 1:L:175:ASP:OD1  | 1:L:177:SER:HB2  | 2.17                     | 0.45              |
| 1:N:30:GLY:HA2   | 1:O:42:LYS:HZ1   | 1.80                     | 0.45              |
| 1:T:142:MET:HE1  | 1:T:149:TYR:CD2  | 2.51                     | 0.45              |
| 1:C:257:MET:HE3  | 1:C:257:MET:HB3  | 1.83                     | 0.45              |
| 1:E:175:ASP:OD1  | 1:E:177:SER:HB2  | 2.17                     | 0.45              |
| 1:E:272:LEU:O    | 1:E:278:GLN:NE2  | 2.46                     | 0.45              |
| 1:I:175:ASP:OD1  | 1:I:177:SER:HB2  | 2.17                     | 0.45              |
| 1:K:364:ASN:O    | 1:K:367:VAL:HG22 | 2.17                     | 0.45              |
| 1:O:175:ASP:OD1  | 1:O:177:SER:HB2  | 2.17                     | 0.45              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:S:175:ASP:OD1 | 1:S:177:SER:HB2  | 2.17                     | 0.45              |
| 1:A:364:ASN:O   | 1:A:367:VAL:HG22 | 2.17                     | 0.45              |
| 1:G:142:MET:HE1 | 1:G:149:TYR:CD2  | 2.51                     | 0.45              |
| 1:Q:142:MET:HE1 | 1:Q:149:TYR:CD2  | 2.51                     | 0.45              |
| 1:H:175:ASP:OD1 | 1:H:177:SER:HB2  | 2.17                     | 0.45              |
| 1:I:142:MET:HE1 | 1:I:149:TYR:CD2  | 2.51                     | 0.45              |
| 1:J:175:ASP:OD1 | 1:J:177:SER:HB2  | 2.17                     | 0.45              |
| 1:M:142:MET:HE1 | 1:M:149:TYR:CD2  | 2.51                     | 0.45              |
| 1:N:175:ASP:OD1 | 1:N:177:SER:HB2  | 2.17                     | 0.45              |
| 1:R:175:ASP:OD1 | 1:R:177:SER:HB2  | 2.17                     | 0.45              |
| 1:S:297:GLU:OE2 | 1:S:301:TYR:OH   | 2.20                     | 0.45              |
| 1:T:175:ASP:OD1 | 1:T:177:SER:HB2  | 2.17                     | 0.45              |
| 1:D:175:ASP:OD1 | 1:D:177:SER:HB2  | 2.17                     | 0.45              |
| 1:D:364:ASN:O   | 1:D:367:VAL:HG22 | 2.17                     | 0.45              |
| 1:F:297:GLU:OE2 | 1:F:301:TYR:OH   | 2.20                     | 0.45              |
| 1:G:354:ALA:HA  | 1:G:357:LEU:HD12 | 1.99                     | 0.45              |
| 1:N:364:ASN:O   | 1:N:367:VAL:HG22 | 2.17                     | 0.45              |
| 1:Q:354:ALA:HA  | 1:Q:357:LEU:HD12 | 1.99                     | 0.45              |
| 1:S:142:MET:HE1 | 1:S:149:TYR:CD2  | 2.51                     | 0.45              |
| 1:C:142:MET:HE1 | 1:C:149:TYR:CD2  | 2.51                     | 0.45              |
| 1:F:30:GLY:HA2  | 1:G:42:LYS:HZ1   | 1.82                     | 0.45              |
| 1:F:354:ALA:HA  | 1:F:357:LEU:HD12 | 1.99                     | 0.45              |
| 1:P:354:ALA:HA  | 1:P:357:LEU:HD12 | 1.99                     | 0.45              |
| 1:Q:175:ASP:OD1 | 1:Q:177:SER:HB2  | 2.17                     | 0.45              |
| 1:G:175:ASP:OD1 | 1:G:177:SER:HB2  | 2.17                     | 0.45              |
| 1:A:142:MET:HE1 | 1:A:149:TYR:CD2  | 2.51                     | 0.45              |
| 1:B:30:GLY:HA2  | 1:C:42:LYS:HZ1   | 1.81                     | 0.45              |
| 1:E:354:ALA:HA  | 1:E:357:LEU:HD12 | 1.99                     | 0.45              |
| 1:H:354:ALA:HA  | 1:H:357:LEU:HD12 | 1.99                     | 0.45              |
| 1:K:142:MET:HE1 | 1:K:149:TYR:CD2  | 2.51                     | 0.45              |
| 1:K:175:ASP:OD1 | 1:K:177:SER:HB2  | 2.17                     | 0.45              |
| 1:M:257:MET:HE3 | 1:M:257:MET:HB3  | 1.83                     | 0.45              |
| 1:O:354:ALA:HA  | 1:O:357:LEU:HD12 | 1.99                     | 0.45              |
| 1:R:354:ALA:HA  | 1:R:357:LEU:HD12 | 1.99                     | 0.45              |
| 1:S:272:LEU:O   | 1:S:278:GLN:NE2  | 2.46                     | 0.45              |
| 1:A:175:ASP:OD1 | 1:A:177:SER:HB2  | 2.17                     | 0.44              |
| 1:C:175:ASP:OD1 | 1:C:177:SER:HB2  | 2.17                     | 0.44              |
| 1:I:297:GLU:OE2 | 1:I:301:TYR:OH   | 2.20                     | 0.44              |
| 1:J:364:ASN:O   | 1:J:367:VAL:HG22 | 2.17                     | 0.44              |
| 1:L:364:ASN:O   | 1:L:367:VAL:HG22 | 2.17                     | 0.44              |
| 1:F:330:GLY:HA3 | 1:F:354:ALA:HB3  | 2.00                     | 0.44              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:I:272:LEU:O   | 1:I:278:GLN:NE2  | 2.46                     | 0.44              |
| 1:M:175:ASP:OD1 | 1:M:177:SER:HB2  | 2.17                     | 0.44              |
| 1:P:330:GLY:HA3 | 1:P:354:ALA:HB3  | 2.00                     | 0.44              |
| 1:B:364:ASN:O   | 1:B:367:VAL:HG22 | 2.17                     | 0.44              |
| 1:T:364:ASN:O   | 1:T:367:VAL:HG22 | 2.17                     | 0.44              |
| 1:C:364:ASN:O   | 1:C:367:VAL:HG22 | 2.17                     | 0.44              |
| 1:E:330:GLY:HA3 | 1:E:354:ALA:HB3  | 2.00                     | 0.44              |
| 1:Q:257:MET:HE3 | 1:Q:257:MET:HB3  | 1.83                     | 0.44              |
| 1:Q:330:GLY:HA3 | 1:Q:354:ALA:HB3  | 2.00                     | 0.44              |
| 1:F:364:ASN:O   | 1:F:367:VAL:HG22 | 2.17                     | 0.44              |
| 1:G:330:GLY:HA3 | 1:G:354:ALA:HB3  | 2.00                     | 0.44              |
| 1:G:364:ASN:O   | 1:G:367:VAL:HG22 | 2.17                     | 0.44              |
| 1:I:354:ALA:HA  | 1:I:357:LEU:HD12 | 1.99                     | 0.44              |
| 1:M:364:ASN:O   | 1:M:367:VAL:HG22 | 2.17                     | 0.44              |
| 1:N:354:ALA:HA  | 1:N:357:LEU:HD12 | 1.99                     | 0.44              |
| 1:O:142:MET:HE1 | 1:O:149:TYR:CD2  | 2.51                     | 0.44              |
| 1:O:330:GLY:HA3 | 1:O:354:ALA:HB3  | 2.00                     | 0.44              |
| 1:D:354:ALA:HA  | 1:D:357:LEU:HD12 | 1.99                     | 0.44              |
| 1:H:364:ASN:O   | 1:H:367:VAL:HG22 | 2.17                     | 0.44              |
| 1:P:364:ASN:O   | 1:P:367:VAL:HG22 | 2.17                     | 0.44              |
| 1:Q:364:ASN:O   | 1:Q:367:VAL:HG22 | 2.17                     | 0.44              |
| 1:S:354:ALA:HA  | 1:S:357:LEU:HD12 | 1.99                     | 0.44              |
| 1:C:354:ALA:HA  | 1:C:357:LEU:HD12 | 1.99                     | 0.44              |
| 1:E:142:MET:HE1 | 1:E:149:TYR:CD2  | 2.51                     | 0.44              |
| 1:J:330:GLY:HA3 | 1:J:354:ALA:HB3  | 2.00                     | 0.44              |
| 1:J:354:ALA:HA  | 1:J:357:LEU:HD12 | 1.99                     | 0.44              |
| 1:M:354:ALA:HA  | 1:M:357:LEU:HD12 | 1.99                     | 0.44              |
| 1:P:175:ASP:OD1 | 1:P:177:SER:HB2  | 2.17                     | 0.44              |
| 1:R:364:ASN:O   | 1:R:367:VAL:HG22 | 2.17                     | 0.44              |
| 1:S:364:ASN:O   | 1:S:367:VAL:HG22 | 2.17                     | 0.44              |
| 1:F:175:ASP:OD1 | 1:F:177:SER:HB2  | 2.17                     | 0.44              |
| 1:I:364:ASN:O   | 1:I:367:VAL:HG22 | 2.17                     | 0.44              |
| 1:N:272:LEU:O   | 1:N:278:GLN:NE2  | 2.46                     | 0.44              |
| 1:T:330:GLY:HA3 | 1:T:354:ALA:HB3  | 2.00                     | 0.44              |
| 1:T:354:ALA:HA  | 1:T:357:LEU:HD12 | 1.99                     | 0.44              |
| 1:A:330:GLY:HA3 | 1:A:354:ALA:HB3  | 2.00                     | 0.44              |
| 1:E:364:ASN:O   | 1:E:367:VAL:HG22 | 2.17                     | 0.44              |
| 1:K:272:LEU:O   | 1:K:278:GLN:NE2  | 2.46                     | 0.44              |
| 1:K:330:GLY:HA3 | 1:K:354:ALA:HB3  | 2.00                     | 0.44              |
| 1:O:364:ASN:O   | 1:O:367:VAL:HG22 | 2.17                     | 0.44              |
| 1:F:135:TYR:CE1 | 1:F:145:VAL:HG11 | 2.54                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:104:ILE:HD11 | 1:L:109:MET:SD   | 2.59                     | 0.43              |
| 1:P:135:TYR:CE1  | 1:P:145:VAL:HG11 | 2.54                     | 0.43              |
| 1:A:354:ALA:HA   | 1:A:357:LEU:HD12 | 1.99                     | 0.43              |
| 1:B:104:ILE:HD11 | 1:B:109:MET:SD   | 2.59                     | 0.43              |
| 1:B:135:TYR:CE1  | 1:B:145:VAL:HG11 | 2.54                     | 0.43              |
| 1:B:354:ALA:HA   | 1:B:357:LEU:HD12 | 1.99                     | 0.43              |
| 1:C:135:TYR:CE1  | 1:C:145:VAL:HG11 | 2.54                     | 0.43              |
| 1:D:272:LEU:O    | 1:D:278:GLN:NE2  | 2.46                     | 0.43              |
| 1:E:34:ASP:HA    | 1:E:93:ASN:HB2   | 2.00                     | 0.43              |
| 1:E:135:TYR:CE1  | 1:E:145:VAL:HG11 | 2.53                     | 0.43              |
| 1:G:104:ILE:HD11 | 1:G:109:MET:SD   | 2.59                     | 0.43              |
| 1:I:135:TYR:CE1  | 1:I:145:VAL:HG11 | 2.54                     | 0.43              |
| 1:J:135:TYR:CE1  | 1:J:145:VAL:HG11 | 2.53                     | 0.43              |
| 1:K:354:ALA:HA   | 1:K:357:LEU:HD12 | 1.99                     | 0.43              |
| 1:L:135:TYR:CE1  | 1:L:145:VAL:HG11 | 2.54                     | 0.43              |
| 1:L:354:ALA:HA   | 1:L:357:LEU:HD12 | 1.99                     | 0.43              |
| 1:M:135:TYR:CE1  | 1:M:145:VAL:HG11 | 2.54                     | 0.43              |
| 1:N:135:TYR:CE1  | 1:N:145:VAL:HG11 | 2.54                     | 0.43              |
| 1:O:34:ASP:HA    | 1:O:93:ASN:HB2   | 2.00                     | 0.43              |
| 1:O:135:TYR:CE1  | 1:O:145:VAL:HG11 | 2.53                     | 0.43              |
| 1:R:330:GLY:HA3  | 1:R:354:ALA:HB3  | 2.00                     | 0.43              |
| 1:S:135:TYR:CE1  | 1:S:145:VAL:HG11 | 2.54                     | 0.43              |
| 1:T:135:TYR:CE1  | 1:T:145:VAL:HG11 | 2.53                     | 0.43              |
| 1:A:272:LEU:O    | 1:A:278:GLN:NE2  | 2.46                     | 0.43              |
| 1:D:135:TYR:CE1  | 1:D:145:VAL:HG11 | 2.54                     | 0.43              |
| 1:H:330:GLY:HA3  | 1:H:354:ALA:HB3  | 2.00                     | 0.43              |
| 1:I:104:ILE:HD11 | 1:I:109:MET:SD   | 2.59                     | 0.43              |
| 1:I:149:TYR:HE1  | 1:I:196:ARG:HG3  | 1.84                     | 0.43              |
| 1:I:330:GLY:HA3  | 1:I:354:ALA:HB3  | 2.00                     | 0.43              |
| 1:Q:104:ILE:HD11 | 1:Q:109:MET:SD   | 2.59                     | 0.43              |
| 1:S:149:TYR:HE1  | 1:S:196:ARG:HG3  | 1.84                     | 0.43              |
| 1:A:104:ILE:HD11 | 1:A:109:MET:SD   | 2.59                     | 0.43              |
| 1:G:149:TYR:HE1  | 1:G:196:ARG:HG3  | 1.84                     | 0.43              |
| 1:K:104:ILE:HD11 | 1:K:109:MET:SD   | 2.59                     | 0.43              |
| 1:N:104:ILE:HD11 | 1:N:109:MET:SD   | 2.59                     | 0.43              |
| 1:Q:149:TYR:HE1  | 1:Q:196:ARG:HG3  | 1.84                     | 0.43              |
| 1:R:135:TYR:CE1  | 1:R:145:VAL:HG11 | 2.54                     | 0.43              |
| 1:S:104:ILE:HD11 | 1:S:109:MET:SD   | 2.59                     | 0.43              |
| 1:T:297:GLU:OE2  | 1:T:301:TYR:OH   | 2.20                     | 0.43              |
| 1:A:135:TYR:CE1  | 1:A:145:VAL:HG11 | 2.54                     | 0.43              |
| 1:B:290:TYR:CZ   | 1:B:294:LEU:HD11 | 2.54                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:34:ASP:HA    | 1:D:93:ASN:HB2   | 2.00                     | 0.43              |
| 1:D:104:ILE:HD11 | 1:D:109:MET:SD   | 2.59                     | 0.43              |
| 1:E:104:ILE:HD11 | 1:E:109:MET:SD   | 2.59                     | 0.43              |
| 1:E:149:TYR:HE1  | 1:E:196:ARG:HG3  | 1.84                     | 0.43              |
| 1:G:135:TYR:CE1  | 1:G:145:VAL:HG11 | 2.54                     | 0.43              |
| 1:H:135:TYR:CE1  | 1:H:145:VAL:HG11 | 2.54                     | 0.43              |
| 1:H:257:MET:HE3  | 1:H:257:MET:HB3  | 1.83                     | 0.43              |
| 1:L:290:TYR:CZ   | 1:L:294:LEU:HD11 | 2.54                     | 0.43              |
| 1:N:34:ASP:HA    | 1:N:93:ASN:HB2   | 2.00                     | 0.43              |
| 1:Q:135:TYR:CE1  | 1:Q:145:VAL:HG11 | 2.54                     | 0.43              |
| 1:S:330:GLY:HA3  | 1:S:354:ALA:HB3  | 2.00                     | 0.43              |
| 1:C:104:ILE:HD11 | 1:C:109:MET:SD   | 2.59                     | 0.43              |
| 1:C:290:TYR:CZ   | 1:C:294:LEU:HD11 | 2.54                     | 0.43              |
| 1:D:330:GLY:HA3  | 1:D:354:ALA:HB3  | 2.00                     | 0.43              |
| 1:H:104:ILE:HD11 | 1:H:109:MET:SD   | 2.59                     | 0.43              |
| 1:K:135:TYR:CE1  | 1:K:145:VAL:HG11 | 2.54                     | 0.43              |
| 1:L:330:GLY:HA3  | 1:L:354:ALA:HB3  | 2.00                     | 0.43              |
| 1:M:290:TYR:CZ   | 1:M:294:LEU:HD11 | 2.54                     | 0.43              |
| 1:O:104:ILE:HD11 | 1:O:109:MET:SD   | 2.59                     | 0.43              |
| 1:O:149:TYR:HE1  | 1:O:196:ARG:HG3  | 1.84                     | 0.43              |
| 1:R:104:ILE:HD11 | 1:R:109:MET:SD   | 2.59                     | 0.43              |
| 1:B:270:ILE:HG22 | 1:C:363:ILE:HG21 | 2.01                     | 0.43              |
| 1:B:330:GLY:HA3  | 1:B:354:ALA:HB3  | 2.00                     | 0.43              |
| 1:E:290:TYR:CZ   | 1:E:294:LEU:HD11 | 2.54                     | 0.43              |
| 1:F:155:ASP:O    | 1:F:159:ILE:HG13 | 2.19                     | 0.43              |
| 1:G:270:ILE:HG22 | 1:H:363:ILE:HG21 | 2.01                     | 0.43              |
| 1:H:149:TYR:HE1  | 1:H:196:ARG:HG3  | 1.84                     | 0.43              |
| 1:J:149:TYR:HE1  | 1:J:196:ARG:HG3  | 1.84                     | 0.43              |
| 1:L:270:ILE:HG22 | 1:M:363:ILE:HG21 | 2.01                     | 0.43              |
| 1:M:104:ILE:HD11 | 1:M:109:MET:SD   | 2.59                     | 0.43              |
| 1:N:330:GLY:HA3  | 1:N:354:ALA:HB3  | 2.00                     | 0.43              |
| 1:O:290:TYR:CZ   | 1:O:294:LEU:HD11 | 2.54                     | 0.43              |
| 1:P:67:MET:HE2   | 1:P:219:PHE:CB   | 2.47                     | 0.43              |
| 1:Q:270:ILE:HG22 | 1:R:363:ILE:HG21 | 2.01                     | 0.43              |
| 1:T:149:TYR:HE1  | 1:T:196:ARG:HG3  | 1.84                     | 0.43              |
| 1:A:149:TYR:HE1  | 1:A:196:ARG:HG3  | 1.84                     | 0.43              |
| 1:D:290:TYR:CZ   | 1:D:294:LEU:HD11 | 2.54                     | 0.43              |
| 1:E:155:ASP:O    | 1:E:159:ILE:HG13 | 2.19                     | 0.43              |
| 1:K:149:TYR:HE1  | 1:K:196:ARG:HG3  | 1.84                     | 0.43              |
| 2:e:1069:C:H2'   | 2:e:1070:C:O4'   | 2.19                     | 0.43              |
| 1:N:290:TYR:CZ   | 1:N:294:LEU:HD11 | 2.54                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:155:ASP:O    | 1:O:159:ILE:HG13 | 2.19                     | 0.43              |
| 1:P:104:ILE:HD11 | 1:P:109:MET:SD   | 2.59                     | 0.43              |
| 1:P:155:ASP:O    | 1:P:159:ILE:HG13 | 2.19                     | 0.43              |
| 1:P:290:TYR:CZ   | 1:P:294:LEU:HD11 | 2.54                     | 0.43              |
| 1:Q:290:TYR:CZ   | 1:Q:294:LEU:HD11 | 2.54                     | 0.43              |
| 1:R:149:TYR:HE1  | 1:R:196:ARG:HG3  | 1.84                     | 0.43              |
| 1:A:270:ILE:HG22 | 1:B:363:ILE:HG21 | 2.01                     | 0.43              |
| 2:U:1069:C:H2'   | 2:U:1070:C:O4'   | 2.19                     | 0.43              |
| 1:B:155:ASP:O    | 1:B:159:ILE:HG13 | 2.19                     | 0.43              |
| 1:C:270:ILE:HG22 | 1:D:363:ILE:HG21 | 2.01                     | 0.43              |
| 1:D:270:ILE:HG22 | 1:E:363:ILE:HG21 | 2.01                     | 0.43              |
| 1:F:67:MET:HE2   | 1:F:219:PHE:CB   | 2.47                     | 0.43              |
| 1:F:104:ILE:HD11 | 1:F:109:MET:SD   | 2.59                     | 0.43              |
| 1:F:270:ILE:HG22 | 1:G:363:ILE:HG21 | 2.01                     | 0.43              |
| 1:F:290:TYR:CZ   | 1:F:294:LEU:HD11 | 2.54                     | 0.43              |
| 1:G:155:ASP:O    | 1:G:159:ILE:HG13 | 2.19                     | 0.43              |
| 1:G:290:TYR:CZ   | 1:G:294:LEU:HD11 | 2.54                     | 0.43              |
| 1:H:270:ILE:HG22 | 1:I:363:ILE:HG21 | 2.01                     | 0.43              |
| 1:I:30:GLY:HA2   | 1:J:42:LYS:HZ1   | 1.83                     | 0.43              |
| 1:I:270:ILE:HG22 | 1:J:363:ILE:HG21 | 2.01                     | 0.43              |
| 1:K:363:ILE:HG21 | 1:T:270:ILE:HG22 | 2.01                     | 0.43              |
| 1:M:270:ILE:HG22 | 1:N:363:ILE:HG21 | 2.01                     | 0.43              |
| 1:N:270:ILE:HG22 | 1:O:363:ILE:HG21 | 2.01                     | 0.43              |
| 1:Q:155:ASP:O    | 1:Q:159:ILE:HG13 | 2.19                     | 0.43              |
| 1:R:270:ILE:HG22 | 1:S:363:ILE:HG21 | 2.01                     | 0.43              |
| 1:S:270:ILE:HG22 | 1:T:363:ILE:HG21 | 2.01                     | 0.43              |
| 1:A:290:TYR:CZ   | 1:A:294:LEU:HD11 | 2.54                     | 0.43              |
| 1:A:363:ILE:HG21 | 1:J:270:ILE:HG22 | 2.01                     | 0.43              |
| 2:U:1062:C:H2'   | 2:U:1063:C:O4'   | 2.19                     | 0.43              |
| 1:H:155:ASP:O    | 1:H:159:ILE:HG13 | 2.19                     | 0.43              |
| 1:J:297:GLU:OE2  | 1:J:301:TYR:OH   | 2.20                     | 0.43              |
| 1:K:270:ILE:HG22 | 1:L:363:ILE:HG21 | 2.01                     | 0.43              |
| 1:K:290:TYR:CZ   | 1:K:294:LEU:HD11 | 2.54                     | 0.43              |
| 2:e:1062:C:H2'   | 2:e:1063:C:O4'   | 2.19                     | 0.43              |
| 1:L:155:ASP:O    | 1:L:159:ILE:HG13 | 2.19                     | 0.43              |
| 1:P:270:ILE:HG22 | 1:Q:363:ILE:HG21 | 2.01                     | 0.43              |
| 1:R:155:ASP:O    | 1:R:159:ILE:HG13 | 2.19                     | 0.43              |
| 1:R:257:MET:HE3  | 1:R:257:MET:HB3  | 1.83                     | 0.43              |
| 1:J:34:ASP:HA    | 1:J:93:ASN:HB2   | 2.00                     | 0.42              |
| 1:K:155:ASP:O    | 1:K:159:ILE:HG13 | 2.19                     | 0.42              |
| 1:O:270:ILE:HG22 | 1:P:363:ILE:HG21 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:30:GLY:HA2   | 1:T:42:LYS:HZ1   | 1.83                     | 0.42              |
| 1:T:34:ASP:HA    | 1:T:93:ASN:HB2   | 2.00                     | 0.42              |
| 1:A:34:ASP:HA    | 1:A:93:ASN:HB2   | 2.00                     | 0.42              |
| 1:A:155:ASP:O    | 1:A:159:ILE:HG13 | 2.19                     | 0.42              |
| 1:C:149:TYR:HE1  | 1:C:196:ARG:HG3  | 1.84                     | 0.42              |
| 1:E:270:ILE:HG22 | 1:F:363:ILE:HG21 | 2.01                     | 0.42              |
| 1:H:166:LEU:O    | 1:H:169:THR:OG1  | 2.32                     | 0.42              |
| 1:J:104:ILE:HD11 | 1:J:109:MET:SD   | 2.59                     | 0.42              |
| 1:J:289:GLU:HA   | 1:J:292:GLN:HG2  | 2.02                     | 0.42              |
| 1:K:34:ASP:HA    | 1:K:93:ASN:HB2   | 2.00                     | 0.42              |
| 2:e:1006:C:H2'   | 2:e:1007:C:O4'   | 2.19                     | 0.42              |
| 2:e:1013:C:H2'   | 2:e:1014:C:O4'   | 2.19                     | 0.42              |
| 1:M:149:TYR:HE1  | 1:M:196:ARG:HG3  | 1.84                     | 0.42              |
| 1:T:104:ILE:HD11 | 1:T:109:MET:SD   | 2.59                     | 0.42              |
| 1:T:289:GLU:HA   | 1:T:292:GLN:HG2  | 2.02                     | 0.42              |
| 2:U:1006:C:H2'   | 2:U:1007:C:O4'   | 2.19                     | 0.42              |
| 2:U:1013:C:H2'   | 2:U:1014:C:O4'   | 2.19                     | 0.42              |
| 1:N:155:ASP:O    | 1:N:159:ILE:HG13 | 2.19                     | 0.42              |
| 1:Q:67:MET:HE2   | 1:Q:219:PHE:CB   | 2.47                     | 0.42              |
| 1:R:272:LEU:O    | 1:R:278:GLN:NE2  | 2.46                     | 0.42              |
| 1:R:290:TYR:CZ   | 1:R:294:LEU:HD11 | 2.54                     | 0.42              |
| 1:S:289:GLU:HA   | 1:S:292:GLN:HG2  | 2.02                     | 0.42              |
| 1:A:289:GLU:HA   | 1:A:292:GLN:HG2  | 2.02                     | 0.42              |
| 1:B:289:GLU:HA   | 1:B:292:GLN:HG2  | 2.02                     | 0.42              |
| 1:D:155:ASP:O    | 1:D:159:ILE:HG13 | 2.19                     | 0.42              |
| 1:F:34:ASP:HA    | 1:F:93:ASN:HB2   | 2.00                     | 0.42              |
| 1:H:290:TYR:CZ   | 1:H:294:LEU:HD11 | 2.54                     | 0.42              |
| 1:I:34:ASP:HA    | 1:I:93:ASN:HB2   | 2.00                     | 0.42              |
| 1:I:155:ASP:O    | 1:I:159:ILE:HG13 | 2.19                     | 0.42              |
| 1:I:289:GLU:HA   | 1:I:292:GLN:HG2  | 2.02                     | 0.42              |
| 1:K:161:LEU:HD23 | 1:K:161:LEU:HA   | 1.82                     | 0.42              |
| 1:K:289:GLU:HA   | 1:K:292:GLN:HG2  | 2.02                     | 0.42              |
| 1:R:166:LEU:O    | 1:R:169:THR:OG1  | 2.32                     | 0.42              |
| 1:R:289:GLU:HA   | 1:R:292:GLN:HG2  | 2.02                     | 0.42              |
| 1:S:34:ASP:HA    | 1:S:93:ASN:HB2   | 2.00                     | 0.42              |
| 1:T:290:TYR:CZ   | 1:T:294:LEU:HD11 | 2.54                     | 0.42              |
| 2:U:1027:C:H2'   | 2:U:1028:C:O4'   | 2.19                     | 0.42              |
| 2:U:1055:C:H2'   | 2:U:1056:C:O4'   | 2.19                     | 0.42              |
| 1:G:67:MET:HE2   | 1:G:219:PHE:CB   | 2.47                     | 0.42              |
| 1:G:166:LEU:O    | 1:G:169:THR:OG1  | 2.32                     | 0.42              |
| 1:G:289:GLU:HA   | 1:G:292:GLN:HG2  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:50:MET:HB3   | 1:H:131:SER:CB   | 2.50                     | 0.42              |
| 1:H:289:GLU:HA   | 1:H:292:GLN:HG2  | 2.02                     | 0.42              |
| 1:I:50:MET:HB3   | 1:I:131:SER:CB   | 2.50                     | 0.42              |
| 1:I:290:TYR:CZ   | 1:I:294:LEU:HD11 | 2.54                     | 0.42              |
| 1:J:290:TYR:CZ   | 1:J:294:LEU:HD11 | 2.54                     | 0.42              |
| 2:e:1055:C:H2'   | 2:e:1056:C:O4'   | 2.19                     | 0.42              |
| 1:L:289:GLU:HA   | 1:L:292:GLN:HG2  | 2.02                     | 0.42              |
| 1:M:330:GLY:HA3  | 1:M:354:ALA:HB3  | 2.00                     | 0.42              |
| 1:Q:289:GLU:HA   | 1:Q:292:GLN:HG2  | 2.02                     | 0.42              |
| 1:R:34:ASP:HA    | 1:R:93:ASN:HB2   | 2.00                     | 0.42              |
| 1:S:50:MET:HB3   | 1:S:131:SER:CB   | 2.50                     | 0.42              |
| 1:S:155:ASP:O    | 1:S:159:ILE:HG13 | 2.19                     | 0.42              |
| 1:S:290:TYR:CZ   | 1:S:294:LEU:HD11 | 2.54                     | 0.42              |
| 1:C:330:GLY:HA3  | 1:C:354:ALA:HB3  | 2.00                     | 0.42              |
| 1:G:50:MET:HB3   | 1:G:131:SER:CB   | 2.50                     | 0.42              |
| 1:H:34:ASP:HA    | 1:H:93:ASN:HB2   | 2.00                     | 0.42              |
| 1:H:272:LEU:O    | 1:H:278:GLN:NE2  | 2.46                     | 0.42              |
| 2:e:1027:C:H2'   | 2:e:1028:C:O4'   | 2.19                     | 0.42              |
| 1:P:34:ASP:HA    | 1:P:93:ASN:HB2   | 2.00                     | 0.42              |
| 1:Q:34:ASP:HA    | 1:Q:93:ASN:HB2   | 2.00                     | 0.42              |
| 1:Q:50:MET:HB3   | 1:Q:131:SER:CB   | 2.50                     | 0.42              |
| 1:R:50:MET:HB3   | 1:R:131:SER:CB   | 2.50                     | 0.42              |
| 1:S:166:LEU:O    | 1:S:169:THR:OG1  | 2.32                     | 0.42              |
| 1:T:50:MET:HB3   | 1:T:131:SER:CB   | 2.50                     | 0.42              |
| 2:U:1034:C:H2'   | 2:U:1035:C:O4'   | 2.19                     | 0.42              |
| 1:F:50:MET:HB3   | 1:F:131:SER:CB   | 2.50                     | 0.42              |
| 1:G:34:ASP:HA    | 1:G:93:ASN:HB2   | 2.00                     | 0.42              |
| 1:J:50:MET:HB3   | 1:J:131:SER:CB   | 2.50                     | 0.42              |
| 1:P:50:MET:HB3   | 1:P:131:SER:CB   | 2.50                     | 0.42              |
| 2:U:1020:C:H2'   | 2:U:1021:C:O4'   | 2.19                     | 0.42              |
| 2:e:1034:C:H2'   | 2:e:1035:C:O4'   | 2.19                     | 0.42              |
| 1:N:67:MET:HE2   | 1:N:219:PHE:CB   | 2.47                     | 0.42              |
| 1:R:67:MET:HE2   | 1:R:219:PHE:CB   | 2.47                     | 0.42              |
| 2:U:1048:C:H2'   | 2:U:1049:C:O4'   | 2.19                     | 0.42              |
| 1:C:155:ASP:O    | 1:C:159:ILE:HG13 | 2.19                     | 0.42              |
| 1:C:289:GLU:HA   | 1:C:292:GLN:HG2  | 2.02                     | 0.42              |
| 1:F:149:TYR:HE1  | 1:F:196:ARG:HG3  | 1.84                     | 0.42              |
| 1:M:34:ASP:HA    | 1:M:93:ASN:HB2   | 2.00                     | 0.42              |
| 1:M:289:GLU:HA   | 1:M:292:GLN:HG2  | 2.02                     | 0.42              |
| 1:P:284:VAL:HG12 | 1:P:317:PHE:CD2  | 2.55                     | 0.42              |
| 1:P:289:GLU:HA   | 1:P:292:GLN:HG2  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:190:LEU:O    | 1:T:194:MET:HG3  | 2.20                     | 0.42              |
| 1:A:161:LEU:HD23 | 1:A:161:LEU:HA   | 1.82                     | 0.42              |
| 2:U:1041:C:H2'   | 2:U:1042:C:O4'   | 2.19                     | 0.42              |
| 1:B:34:ASP:HA    | 1:B:93:ASN:HB2   | 2.00                     | 0.42              |
| 1:C:190:LEU:O    | 1:C:194:MET:HG3  | 2.20                     | 0.42              |
| 1:D:67:MET:HE2   | 1:D:219:PHE:CB   | 2.47                     | 0.42              |
| 1:E:50:MET:HB3   | 1:E:131:SER:CB   | 2.50                     | 0.42              |
| 1:F:284:VAL:HG12 | 1:F:317:PHE:CD2  | 2.55                     | 0.42              |
| 1:F:289:GLU:HA   | 1:F:292:GLN:HG2  | 2.02                     | 0.42              |
| 1:J:190:LEU:O    | 1:J:194:MET:HG3  | 2.20                     | 0.42              |
| 1:K:50:MET:HB3   | 1:K:131:SER:CB   | 2.50                     | 0.42              |
| 2:e:1020:C:H2'   | 2:e:1021:C:O4'   | 2.19                     | 0.42              |
| 2:e:1048:C:H2'   | 2:e:1049:C:O4'   | 2.19                     | 0.42              |
| 1:L:34:ASP:HA    | 1:L:93:ASN:HB2   | 2.00                     | 0.42              |
| 1:N:149:TYR:HE1  | 1:N:196:ARG:HG3  | 1.84                     | 0.42              |
| 1:O:67:MET:HE2   | 1:O:219:PHE:CB   | 2.47                     | 0.42              |
| 1:O:289:GLU:HA   | 1:O:292:GLN:HG2  | 2.02                     | 0.42              |
| 1:A:50:MET:HB3   | 1:A:131:SER:CB   | 2.50                     | 0.41              |
| 1:D:190:LEU:O    | 1:D:194:MET:HG3  | 2.20                     | 0.41              |
| 1:E:289:GLU:HA   | 1:E:292:GLN:HG2  | 2.02                     | 0.41              |
| 1:H:67:MET:HE2   | 1:H:219:PHE:CB   | 2.47                     | 0.41              |
| 1:I:190:LEU:O    | 1:I:194:MET:HG3  | 2.20                     | 0.41              |
| 2:e:1041:C:H2'   | 2:e:1042:C:O4'   | 2.19                     | 0.41              |
| 1:M:155:ASP:O    | 1:M:159:ILE:HG13 | 2.19                     | 0.41              |
| 1:M:190:LEU:O    | 1:M:194:MET:HG3  | 2.20                     | 0.41              |
| 1:N:190:LEU:O    | 1:N:194:MET:HG3  | 2.20                     | 0.41              |
| 1:O:50:MET:HB3   | 1:O:131:SER:CB   | 2.50                     | 0.41              |
| 1:P:149:TYR:HE1  | 1:P:196:ARG:HG3  | 1.84                     | 0.41              |
| 2:U:1058:C:H2'   | 2:U:1059:C:O4'   | 2.20                     | 0.41              |
| 1:C:34:ASP:HA    | 1:C:93:ASN:HB2   | 2.00                     | 0.41              |
| 1:D:149:TYR:HE1  | 1:D:196:ARG:HG3  | 1.84                     | 0.41              |
| 1:D:284:VAL:HG12 | 1:D:317:PHE:CD2  | 2.55                     | 0.41              |
| 1:D:289:GLU:HA   | 1:D:292:GLN:HG2  | 2.02                     | 0.41              |
| 1:E:67:MET:HE2   | 1:E:219:PHE:CB   | 2.47                     | 0.41              |
| 1:G:30:GLY:HA2   | 1:H:42:LYS:HZ1   | 1.84                     | 0.41              |
| 2:e:1058:C:H2'   | 2:e:1059:C:O4'   | 2.20                     | 0.41              |
| 1:N:289:GLU:HA   | 1:N:292:GLN:HG2  | 2.02                     | 0.41              |
| 1:S:190:LEU:O    | 1:S:194:MET:HG3  | 2.20                     | 0.41              |
| 1:T:155:ASP:O    | 1:T:159:ILE:HG13 | 2.19                     | 0.41              |
| 1:A:190:LEU:O    | 1:A:194:MET:HG3  | 2.20                     | 0.41              |
| 2:U:1044:C:H2'   | 2:U:1045:C:O4'   | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:30:GLY:HA2   | 1:D:42:LYS:HZ1   | 1.84                     | 0.41              |
| 1:C:150:ARG:HD3  | 1:C:152:ASP:HB2  | 2.03                     | 0.41              |
| 1:G:284:VAL:HG12 | 1:G:317:PHE:CD2  | 2.55                     | 0.41              |
| 1:J:155:ASP:O    | 1:J:159:ILE:HG13 | 2.19                     | 0.41              |
| 1:K:190:LEU:O    | 1:K:194:MET:HG3  | 2.20                     | 0.41              |
| 2:e:1044:C:H2'   | 2:e:1045:C:O4'   | 2.20                     | 0.41              |
| 2:e:1065:C:H2'   | 2:e:1066:C:O4'   | 2.20                     | 0.41              |
| 1:L:149:TYR:HE1  | 1:L:196:ARG:HG3  | 1.84                     | 0.41              |
| 1:M:150:ARG:HD3  | 1:M:152:ASP:HB2  | 2.03                     | 0.41              |
| 1:N:284:VAL:HG12 | 1:N:317:PHE:CD2  | 2.55                     | 0.41              |
| 1:A:221:ASP:OD1  | 1:B:234:ARG:NH2  | 2.47                     | 0.41              |
| 2:U:1037:C:H2'   | 2:U:1038:C:O4'   | 2.21                     | 0.41              |
| 2:U:1051:C:H2'   | 2:U:1052:C:O4'   | 2.20                     | 0.41              |
| 2:U:1065:C:H2'   | 2:U:1066:C:O4'   | 2.20                     | 0.41              |
| 1:B:149:TYR:HE1  | 1:B:196:ARG:HG3  | 1.84                     | 0.41              |
| 1:B:150:ARG:HD3  | 1:B:152:ASP:HB2  | 2.03                     | 0.41              |
| 1:I:284:VAL:HG12 | 1:I:317:PHE:CD2  | 2.55                     | 0.41              |
| 1:J:166:LEU:O    | 1:J:169:THR:OG1  | 2.32                     | 0.41              |
| 2:e:1037:C:H2'   | 2:e:1038:C:O4'   | 2.21                     | 0.41              |
| 1:M:67:MET:HE2   | 1:M:219:PHE:CB   | 2.47                     | 0.41              |
| 1:N:150:ARG:HD3  | 1:N:152:ASP:HB2  | 2.03                     | 0.41              |
| 1:S:284:VAL:HG12 | 1:S:317:PHE:CD2  | 2.55                     | 0.41              |
| 1:A:284:VAL:HG12 | 1:A:317:PHE:CD2  | 2.55                     | 0.41              |
| 1:B:257:MET:HB3  | 1:B:257:MET:HE3  | 1.83                     | 0.41              |
| 1:C:67:MET:HE2   | 1:C:219:PHE:CB   | 2.47                     | 0.41              |
| 1:D:50:MET:HB3   | 1:D:131:SER:CB   | 2.50                     | 0.41              |
| 1:D:150:ARG:HD3  | 1:D:152:ASP:HB2  | 2.03                     | 0.41              |
| 1:E:257:MET:HE3  | 1:E:257:MET:HB3  | 1.83                     | 0.41              |
| 1:K:284:VAL:HG12 | 1:K:317:PHE:CD2  | 2.55                     | 0.41              |
| 2:e:1051:C:H2'   | 2:e:1052:C:O4'   | 2.20                     | 0.41              |
| 1:L:50:MET:HB3   | 1:L:131:SER:CB   | 2.50                     | 0.41              |
| 1:L:150:ARG:HD3  | 1:L:152:ASP:HB2  | 2.03                     | 0.41              |
| 1:P:171:LEU:HD23 | 1:P:171:LEU:HA   | 1.94                     | 0.41              |
| 1:Q:284:VAL:HG12 | 1:Q:317:PHE:CD2  | 2.55                     | 0.41              |
| 1:B:50:MET:HB3   | 1:B:131:SER:CB   | 2.50                     | 0.41              |
| 1:D:161:LEU:HA   | 1:D:161:LEU:HD23 | 1.82                     | 0.41              |
| 1:F:149:TYR:CE1  | 1:F:196:ARG:HA   | 2.55                     | 0.41              |
| 1:F:171:LEU:HD23 | 1:F:171:LEU:HA   | 1.94                     | 0.41              |
| 1:N:50:MET:HB3   | 1:N:131:SER:CB   | 2.50                     | 0.41              |
| 1:R:284:VAL:HG12 | 1:R:317:PHE:CD2  | 2.55                     | 0.41              |
| 1:S:67:MET:HE2   | 1:S:219:PHE:CB   | 2.47                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:190:LEU:O    | 1:B:194:MET:HG3  | 2.20                     | 0.41              |
| 1:C:50:MET:HB3   | 1:C:131:SER:CB   | 2.50                     | 0.41              |
| 1:F:190:LEU:O    | 1:F:194:MET:HG3  | 2.20                     | 0.41              |
| 1:M:50:MET:HB3   | 1:M:131:SER:CB   | 2.50                     | 0.41              |
| 1:G:330:GLY:O    | 1:G:358:LYS:NZ   | 2.54                     | 0.41              |
| 1:H:284:VAL:HG12 | 1:H:317:PHE:CD2  | 2.55                     | 0.41              |
| 1:L:190:LEU:O    | 1:L:194:MET:HG3  | 2.20                     | 0.41              |
| 1:O:190:LEU:O    | 1:O:194:MET:HG3  | 2.20                     | 0.41              |
| 1:O:284:VAL:HG12 | 1:O:317:PHE:CD2  | 2.55                     | 0.41              |
| 1:P:190:LEU:O    | 1:P:194:MET:HG3  | 2.20                     | 0.41              |
| 1:Q:330:GLY:O    | 1:Q:358:LYS:NZ   | 2.54                     | 0.41              |
| 1:C:284:VAL:HG12 | 1:C:317:PHE:CD2  | 2.55                     | 0.41              |
| 1:E:190:LEU:O    | 1:E:194:MET:HG3  | 2.20                     | 0.41              |
| 1:E:284:VAL:HG12 | 1:E:317:PHE:CD2  | 2.55                     | 0.41              |
| 1:F:166:LEU:O    | 1:F:169:THR:OG1  | 2.32                     | 0.41              |
| 1:F:330:GLY:O    | 1:F:358:LYS:NZ   | 2.54                     | 0.41              |
| 1:H:190:LEU:O    | 1:H:194:MET:HG3  | 2.20                     | 0.41              |
| 1:H:330:GLY:O    | 1:H:358:LYS:NZ   | 2.54                     | 0.41              |
| 1:I:67:MET:HE2   | 1:I:219:PHE:CB   | 2.47                     | 0.41              |
| 1:M:284:VAL:HG12 | 1:M:317:PHE:CD2  | 2.55                     | 0.41              |
| 1:N:161:LEU:HA   | 1:N:161:LEU:HD23 | 1.82                     | 0.41              |
| 1:O:149:TYR:CE1  | 1:O:196:ARG:HA   | 2.55                     | 0.41              |
| 1:O:150:ARG:HD3  | 1:O:152:ASP:HB2  | 2.03                     | 0.41              |
| 1:P:330:GLY:O    | 1:P:358:LYS:NZ   | 2.54                     | 0.41              |
| 1:Q:161:LEU:HD23 | 1:Q:161:LEU:HA   | 1.82                     | 0.41              |
| 1:R:330:GLY:O    | 1:R:358:LYS:NZ   | 2.54                     | 0.41              |
| 1:T:284:VAL:HG12 | 1:T:317:PHE:CD2  | 2.55                     | 0.41              |
| 1:E:149:TYR:CE1  | 1:E:196:ARG:HA   | 2.55                     | 0.41              |
| 1:J:284:VAL:HG12 | 1:J:317:PHE:CD2  | 2.55                     | 0.41              |
| 1:O:257:MET:HB3  | 1:O:257:MET:HE3  | 1.83                     | 0.41              |
| 1:R:190:LEU:O    | 1:R:194:MET:HG3  | 2.20                     | 0.41              |
| 1:A:30:GLY:HA2   | 1:B:42:LYS:HZ1   | 1.86                     | 0.40              |
| 1:A:150:ARG:HD3  | 1:A:152:ASP:HB2  | 2.03                     | 0.40              |
| 1:E:150:ARG:HD3  | 1:E:152:ASP:HB2  | 2.03                     | 0.40              |
| 1:E:161:LEU:HD23 | 1:E:161:LEU:HA   | 1.82                     | 0.40              |
| 1:I:330:GLY:O    | 1:I:358:LYS:NZ   | 2.54                     | 0.40              |
| 1:M:272:LEU:O    | 1:M:278:GLN:NE2  | 2.46                     | 0.40              |
| 1:O:161:LEU:HD23 | 1:O:161:LEU:HA   | 1.82                     | 0.40              |
| 1:S:330:GLY:O    | 1:S:358:LYS:NZ   | 2.54                     | 0.40              |
| 1:B:284:VAL:HG12 | 1:B:317:PHE:CD2  | 2.55                     | 0.40              |
| 1:B:330:GLY:O    | 1:B:358:LYS:NZ   | 2.54                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:190:LEU:O    | 1:G:194:MET:HG3  | 2.20                     | 0.40              |
| 1:G:221:ASP:OD1  | 1:H:234:ARG:NH2  | 2.47                     | 0.40              |
| 1:J:149:TYR:CE1  | 1:J:196:ARG:HA   | 2.55                     | 0.40              |
| 2:e:1016:C:H2'   | 2:e:1017:C:O4'   | 2.20                     | 0.40              |
| 1:L:67:MET:HE2   | 1:L:219:PHE:CB   | 2.47                     | 0.40              |
| 1:L:284:VAL:HG12 | 1:L:317:PHE:CD2  | 2.55                     | 0.40              |
| 1:A:367:VAL:HG23 | 1:A:368:LEU:HD12 | 2.04                     | 0.40              |
| 2:U:1016:C:H2'   | 2:U:1017:C:O4'   | 2.20                     | 0.40              |
| 1:B:67:MET:HE2   | 1:B:219:PHE:CB   | 2.47                     | 0.40              |
| 1:E:330:GLY:O    | 1:E:358:LYS:NZ   | 2.54                     | 0.40              |
| 1:H:161:LEU:HA   | 1:H:161:LEU:HD23 | 1.82                     | 0.40              |
| 1:I:29:THR:HG23  | 1:I:88:TYR:HB3   | 2.04                     | 0.40              |
| 1:K:150:ARG:HD3  | 1:K:152:ASP:HB2  | 2.03                     | 0.40              |
| 1:L:330:GLY:O    | 1:L:358:LYS:NZ   | 2.54                     | 0.40              |
| 1:Q:272:LEU:O    | 1:Q:278:GLN:NE2  | 2.46                     | 0.40              |
| 1:S:29:THR:HG23  | 1:S:88:TYR:HB3   | 2.04                     | 0.40              |
| 2:U:1009:C:H2'   | 2:U:1010:C:O4'   | 2.20                     | 0.40              |
| 1:C:272:LEU:O    | 1:C:278:GLN:NE2  | 2.46                     | 0.40              |
| 1:G:150:ARG:HD3  | 1:G:152:ASP:HB2  | 2.03                     | 0.40              |
| 1:H:150:ARG:HD3  | 1:H:152:ASP:HB2  | 2.03                     | 0.40              |
| 1:I:168:ILE:HG13 | 1:I:223:PHE:CE2  | 2.57                     | 0.40              |
| 1:J:330:GLY:O    | 1:J:358:LYS:NZ   | 2.54                     | 0.40              |
| 1:K:367:VAL:HG23 | 1:K:368:LEU:HD12 | 2.04                     | 0.40              |
| 2:e:1002:C:H2'   | 2:e:1003:C:O4'   | 2.21                     | 0.40              |
| 1:L:257:MET:HE3  | 1:L:257:MET:HB3  | 1.83                     | 0.40              |
| 1:N:149:TYR:CE1  | 1:N:196:ARG:HA   | 2.55                     | 0.40              |
| 1:O:330:GLY:O    | 1:O:358:LYS:NZ   | 2.54                     | 0.40              |
| 1:Q:190:LEU:O    | 1:Q:194:MET:HG3  | 2.20                     | 0.40              |
| 1:R:150:ARG:HD3  | 1:R:152:ASP:HB2  | 2.03                     | 0.40              |
| 2:U:1002:C:H2'   | 2:U:1003:C:O4'   | 2.21                     | 0.40              |
| 1:B:367:VAL:HG23 | 1:B:368:LEU:HD12 | 2.04                     | 0.40              |
| 1:H:29:THR:HG23  | 1:H:88:TYR:HB3   | 2.04                     | 0.40              |
| 1:J:367:VAL:HG23 | 1:J:368:LEU:HD12 | 2.04                     | 0.40              |
| 2:e:1009:C:H2'   | 2:e:1010:C:O4'   | 2.20                     | 0.40              |
| 1:L:367:VAL:HG23 | 1:L:368:LEU:HD12 | 2.04                     | 0.40              |
| 1:Q:150:ARG:HD3  | 1:Q:152:ASP:HB2  | 2.03                     | 0.40              |
| 1:S:168:ILE:HG13 | 1:S:223:PHE:CE2  | 2.57                     | 0.40              |
| 1:T:67:MET:HE2   | 1:T:219:PHE:CB   | 2.47                     | 0.40              |
| 1:T:330:GLY:O    | 1:T:358:LYS:NZ   | 2.54                     | 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     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | B     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | C     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | D     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | E     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | F     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | G     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | H     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | I     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | J     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | K     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | L     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | M     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | N     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | O     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | P     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | Q     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | R     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | S     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| 1   | T     | 377/391 (96%)   | 368 (98%)  | 9 (2%)   | 0        | 100         | 100 |
| All | All   | 7540/7820 (96%) | 7360 (98%) | 180 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | B     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | C     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | D     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | E     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | F     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | G     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | H     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | I     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | J     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | K     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | L     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | M     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | N     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | O     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | P     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | Q     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | R     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | S     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| 1   | T     | 316/328 (96%)   | 316 (100%)  | 0        | 100         | 100 |
| All | All   | 6320/6560 (96%) | 6320 (100%) | 0        | 100         | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 102 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 216 | HIS  |
| 1   | A     | 316 | GLN  |
| 1   | B     | 41  | GLN  |
| 1   | B     | 102 | GLN  |
| 1   | B     | 151 | HIS  |
| 1   | B     | 192 | ASN  |
| 1   | B     | 216 | HIS  |
| 1   | B     | 316 | GLN  |
| 1   | C     | 151 | HIS  |
| 1   | C     | 216 | HIS  |
| 1   | C     | 316 | GLN  |
| 1   | D     | 102 | GLN  |
| 1   | D     | 216 | HIS  |
| 1   | D     | 316 | GLN  |
| 1   | E     | 102 | GLN  |
| 1   | E     | 192 | ASN  |
| 1   | E     | 216 | HIS  |
| 1   | E     | 316 | GLN  |
| 1   | F     | 216 | HIS  |
| 1   | F     | 316 | GLN  |
| 1   | G     | 41  | GLN  |
| 1   | G     | 102 | GLN  |
| 1   | G     | 151 | HIS  |
| 1   | G     | 216 | HIS  |
| 1   | G     | 316 | GLN  |
| 1   | H     | 216 | HIS  |
| 1   | H     | 316 | GLN  |
| 1   | I     | 151 | HIS  |
| 1   | I     | 216 | HIS  |
| 1   | I     | 316 | GLN  |
| 1   | J     | 102 | GLN  |
| 1   | J     | 151 | HIS  |
| 1   | J     | 192 | ASN  |
| 1   | J     | 216 | HIS  |
| 1   | J     | 316 | GLN  |
| 1   | K     | 102 | GLN  |
| 1   | K     | 216 | HIS  |
| 1   | K     | 316 | GLN  |
| 1   | L     | 41  | GLN  |
| 1   | L     | 102 | GLN  |
| 1   | L     | 151 | HIS  |
| 1   | L     | 192 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 216 | HIS  |
| 1   | L     | 316 | GLN  |
| 1   | M     | 151 | HIS  |
| 1   | M     | 216 | HIS  |
| 1   | M     | 316 | GLN  |
| 1   | N     | 102 | GLN  |
| 1   | N     | 192 | ASN  |
| 1   | N     | 216 | HIS  |
| 1   | N     | 316 | GLN  |
| 1   | O     | 102 | GLN  |
| 1   | O     | 192 | ASN  |
| 1   | O     | 216 | HIS  |
| 1   | O     | 316 | GLN  |
| 1   | P     | 216 | HIS  |
| 1   | P     | 316 | GLN  |
| 1   | Q     | 41  | GLN  |
| 1   | Q     | 102 | GLN  |
| 1   | Q     | 151 | HIS  |
| 1   | Q     | 216 | HIS  |
| 1   | Q     | 316 | GLN  |
| 1   | R     | 102 | GLN  |
| 1   | R     | 216 | HIS  |
| 1   | R     | 316 | GLN  |
| 1   | S     | 151 | HIS  |
| 1   | S     | 216 | HIS  |
| 1   | S     | 316 | GLN  |
| 1   | T     | 151 | HIS  |
| 1   | T     | 192 | ASN  |
| 1   | T     | 216 | HIS  |
| 1   | T     | 316 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed      | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 2   | U     | 69/70 (98%)   | 9 (13%)           | 0               |
| 2   | e     | 69/70 (98%)   | 9 (13%)           | 0               |
| All | All   | 138/140 (98%) | 18 (13%)          | 0               |

All (18) RNA backbone outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | U     | 1008 | C    |
| 2   | U     | 1015 | C    |
| 2   | U     | 1022 | C    |
| 2   | U     | 1029 | C    |
| 2   | U     | 1036 | C    |
| 2   | U     | 1043 | C    |
| 2   | U     | 1050 | C    |
| 2   | U     | 1057 | C    |
| 2   | U     | 1064 | C    |
| 2   | e     | 1008 | C    |
| 2   | e     | 1015 | C    |
| 2   | e     | 1022 | C    |
| 2   | e     | 1029 | C    |
| 2   | e     | 1036 | C    |
| 2   | e     | 1043 | C    |
| 2   | e     | 1050 | C    |
| 2   | e     | 1057 | C    |
| 2   | e     | 1064 | C    |

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2   | U     | 9                |
| 2   | e     | 9                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | U     | 1007:C    | O3'    | 1008:C    | P      | 2.82         |
| 1     | U     | 1014:C    | O3'    | 1015:C    | P      | 2.82         |
| 1     | U     | 1021:C    | O3'    | 1022:C    | P      | 2.82         |
| 1     | U     | 1028:C    | O3'    | 1029:C    | P      | 2.82         |
| 1     | U     | 1035:C    | O3'    | 1036:C    | P      | 2.82         |
| 1     | U     | 1042:C    | O3'    | 1043:C    | P      | 2.82         |
| 1     | U     | 1049:C    | O3'    | 1050:C    | P      | 2.82         |
| 1     | U     | 1056:C    | O3'    | 1057:C    | P      | 2.82         |
| 1     | U     | 1063:C    | O3'    | 1064:C    | P      | 2.82         |
| 1     | e     | 1007:C    | O3'    | 1008:C    | P      | 2.82         |
| 1     | e     | 1014:C    | O3'    | 1015:C    | P      | 2.82         |
| 1     | e     | 1021:C    | O3'    | 1022:C    | P      | 2.82         |
| 1     | e     | 1028:C    | O3'    | 1029:C    | P      | 2.82         |
| 1     | e     | 1035:C    | O3'    | 1036:C    | P      | 2.82         |
| 1     | e     | 1042:C    | O3'    | 1043:C    | P      | 2.82         |
| 1     | e     | 1049:C    | O3'    | 1050:C    | P      | 2.82         |
| 1     | e     | 1056:C    | O3'    | 1057:C    | P      | 2.82         |
| 1     | e     | 1063:C    | O3'    | 1064:C    | P      | 2.82         |

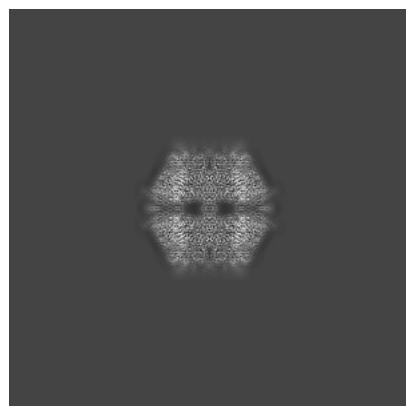
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17031. These allow visual inspection of the internal detail of the map and identification of artifacts.

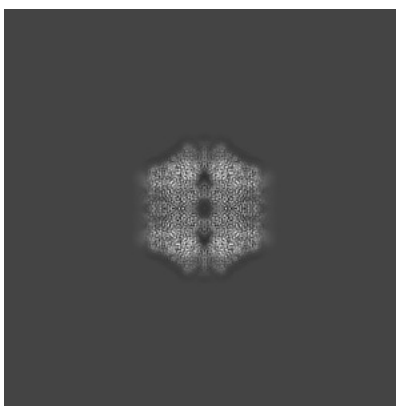
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

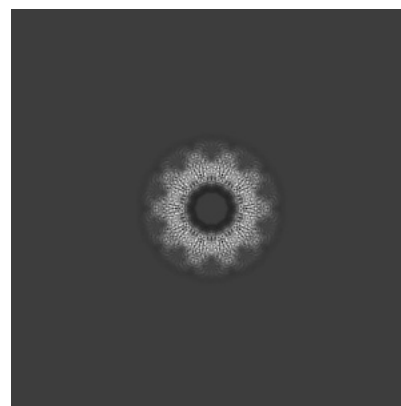
#### 6.1.1 Primary map



X

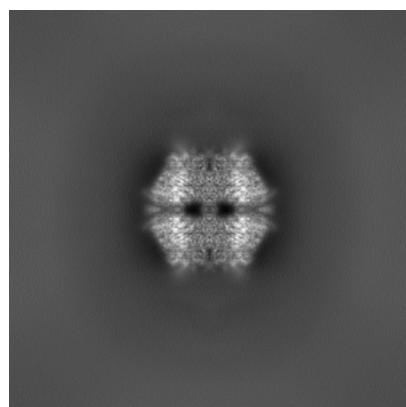


Y

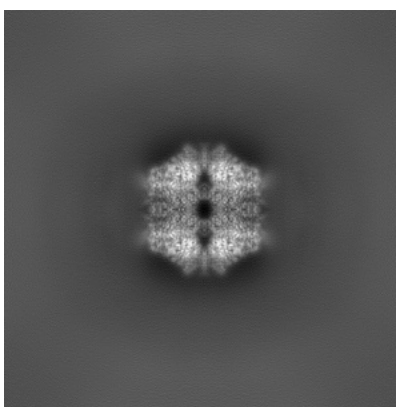


Z

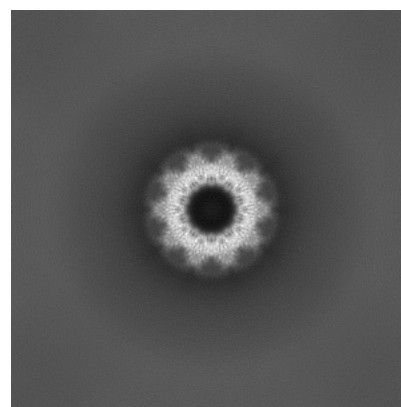
#### 6.1.2 Raw map



X



Y



Z

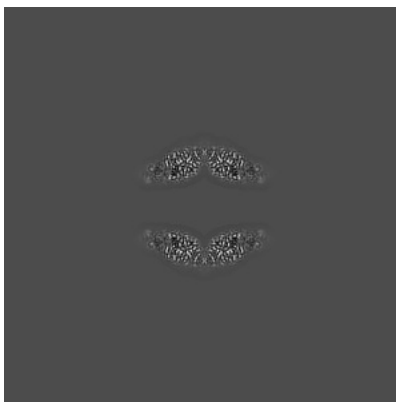
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

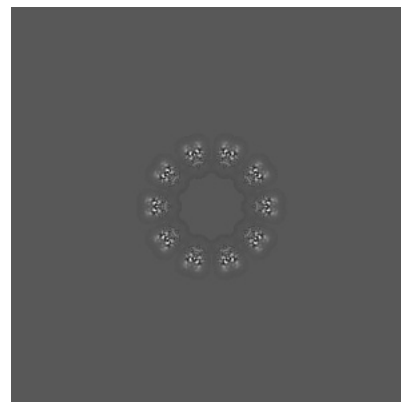
### 6.2.1 Primary map



X Index: 220

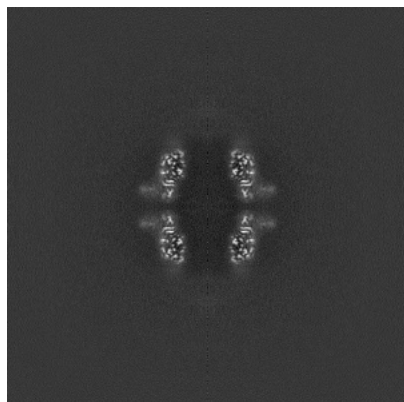


Y Index: 220

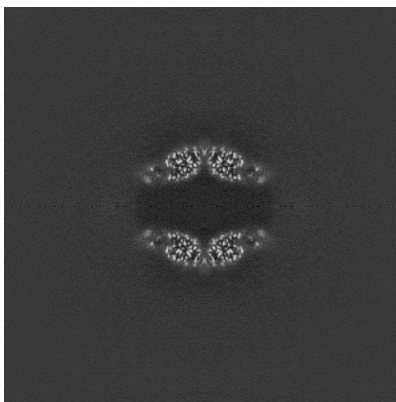


Z Index: 220

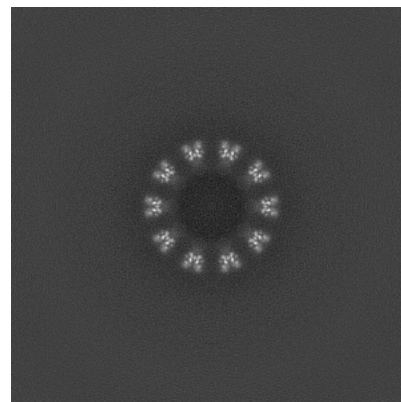
### 6.2.2 Raw map



X Index: 220



Y Index: 220

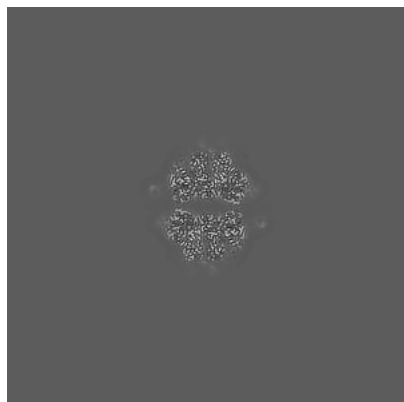


Z Index: 220

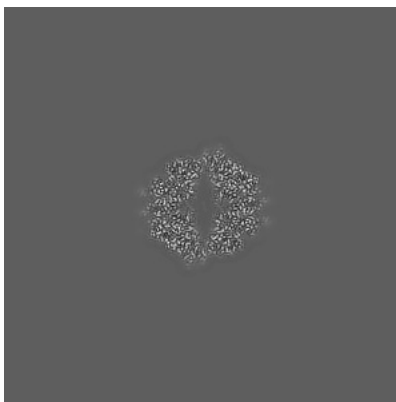
The images above show central slices of the map in three orthogonal directions.

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

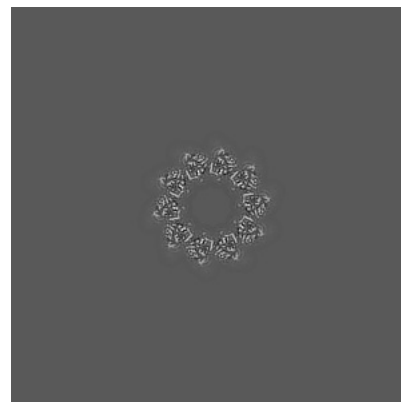
### 6.3.1 Primary map



X Index: 181

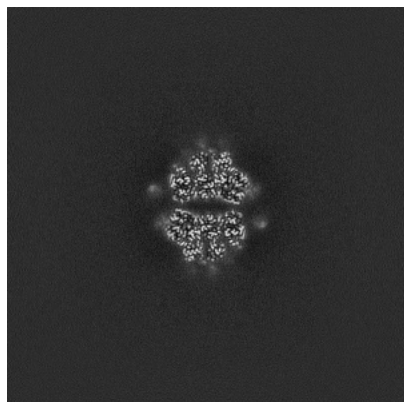


Y Index: 253

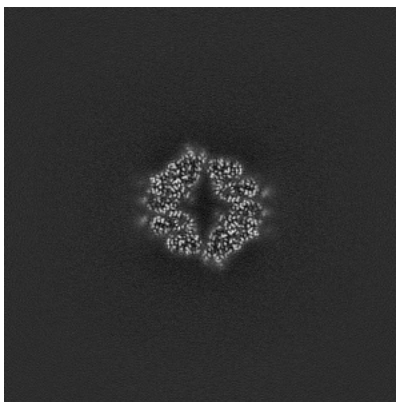


Z Index: 196

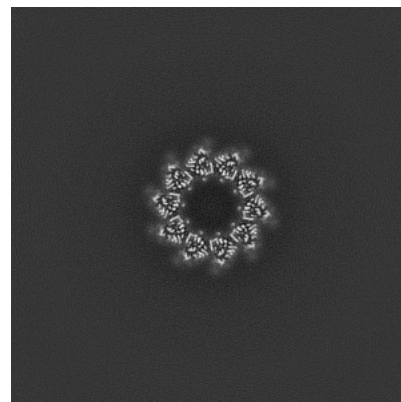
### 6.3.2 Raw map



X Index: 181



Y Index: 188

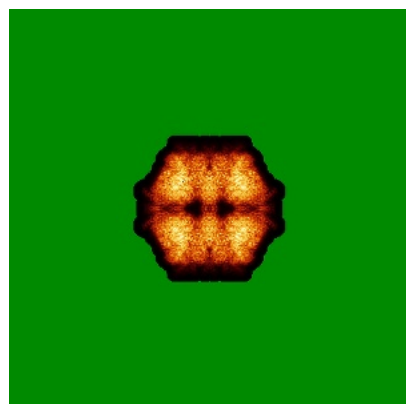


Z Index: 244

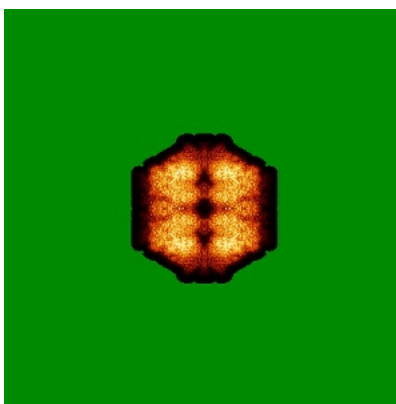
The images above show the largest variance slices of the map in three orthogonal directions.

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

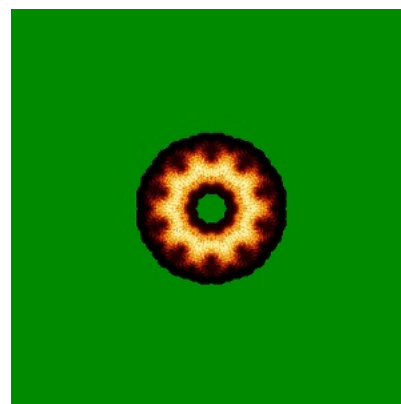
### 6.4.1 Primary map



X

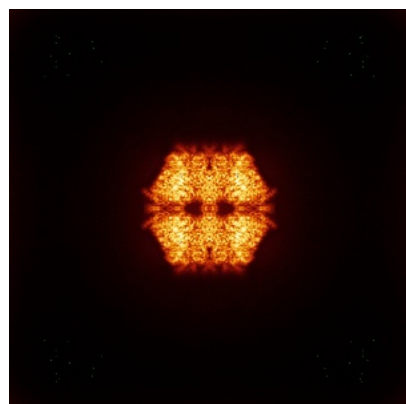


Y

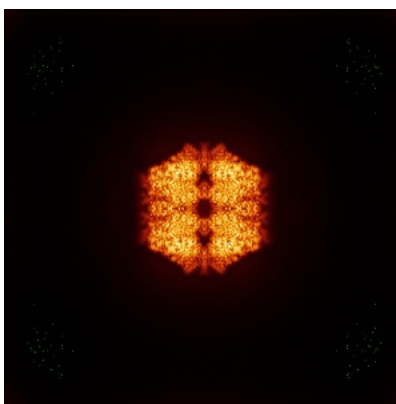


Z

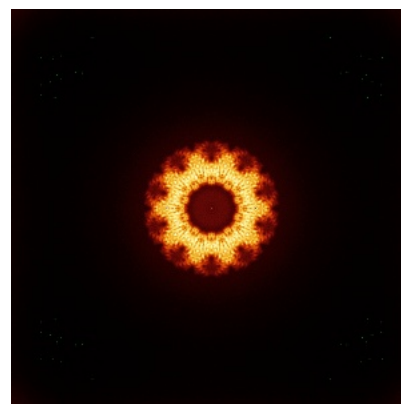
### 6.4.2 Raw map



X



Y

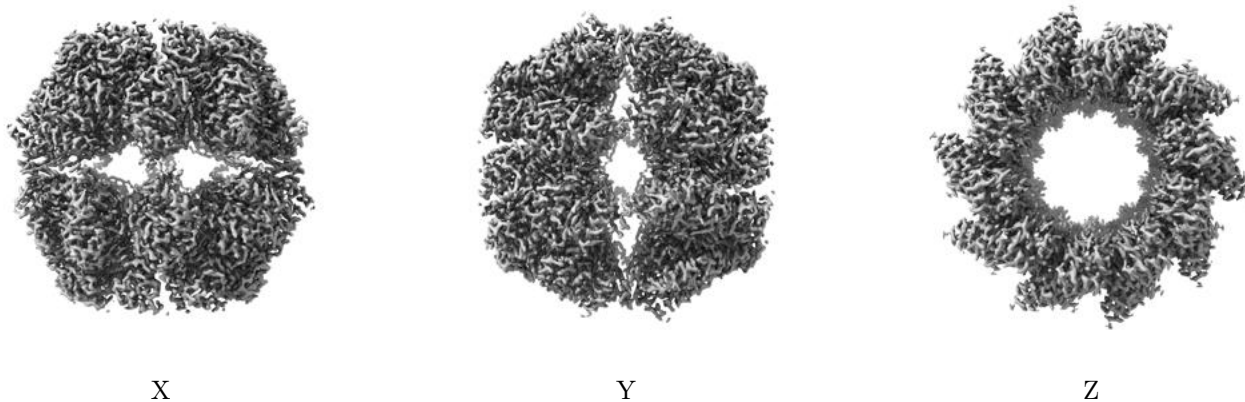


Z

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

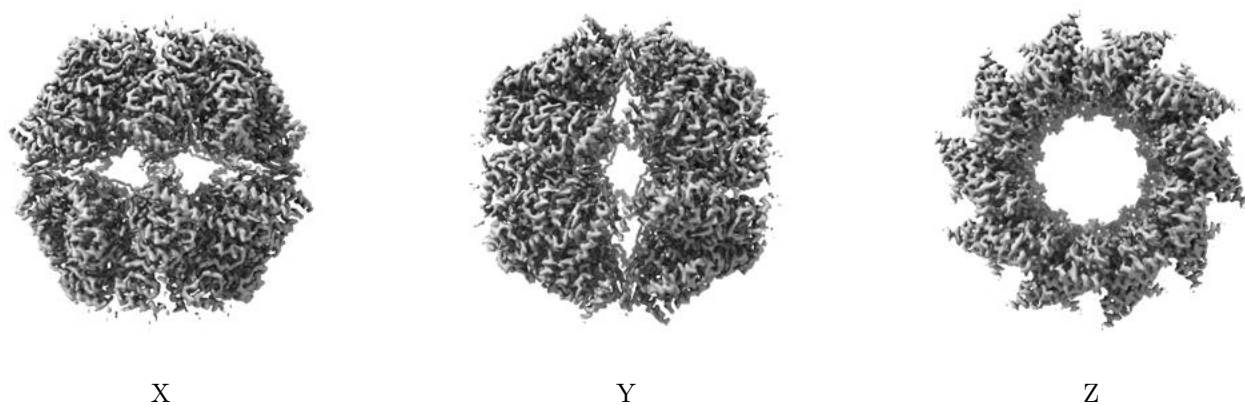
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

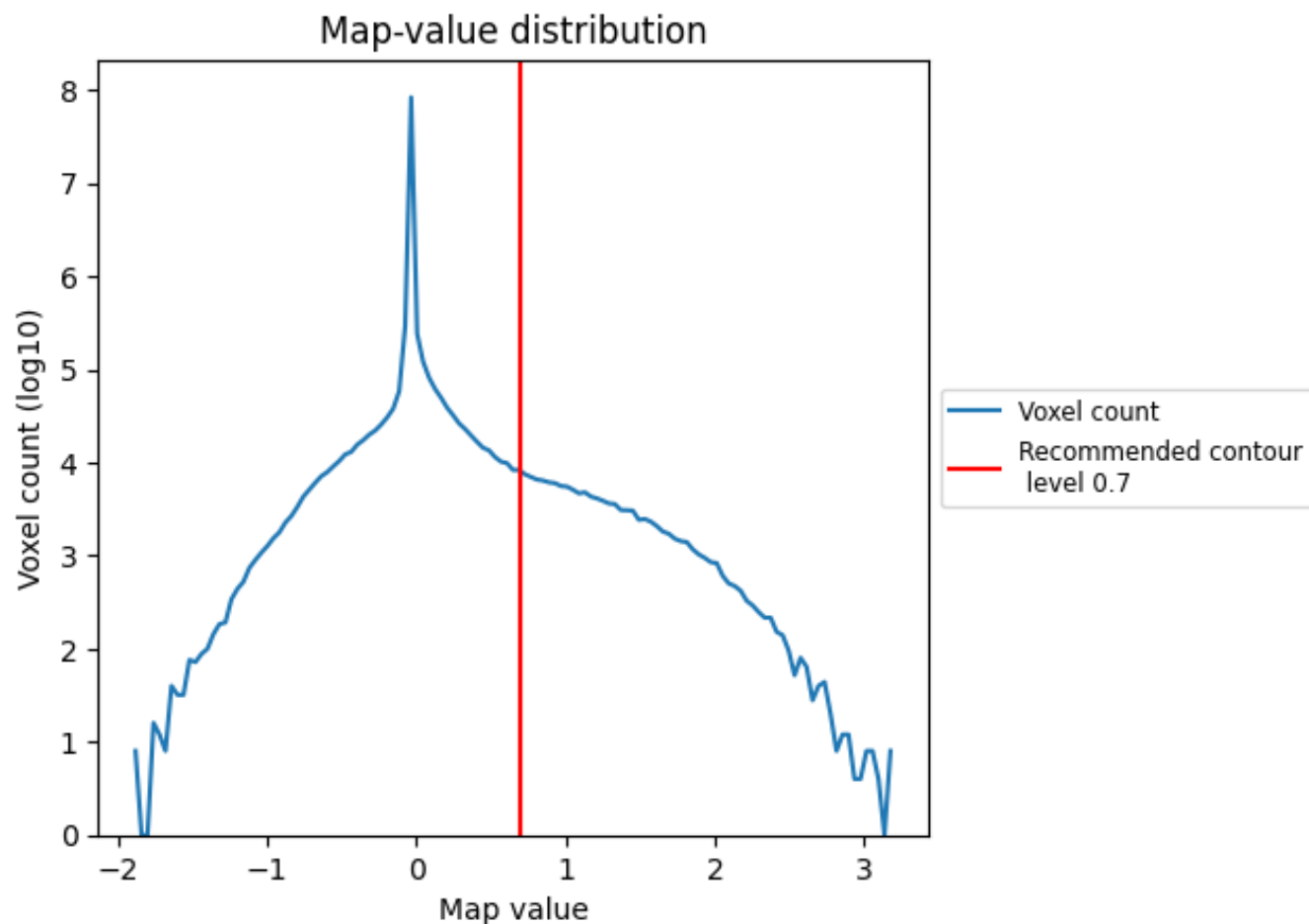
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

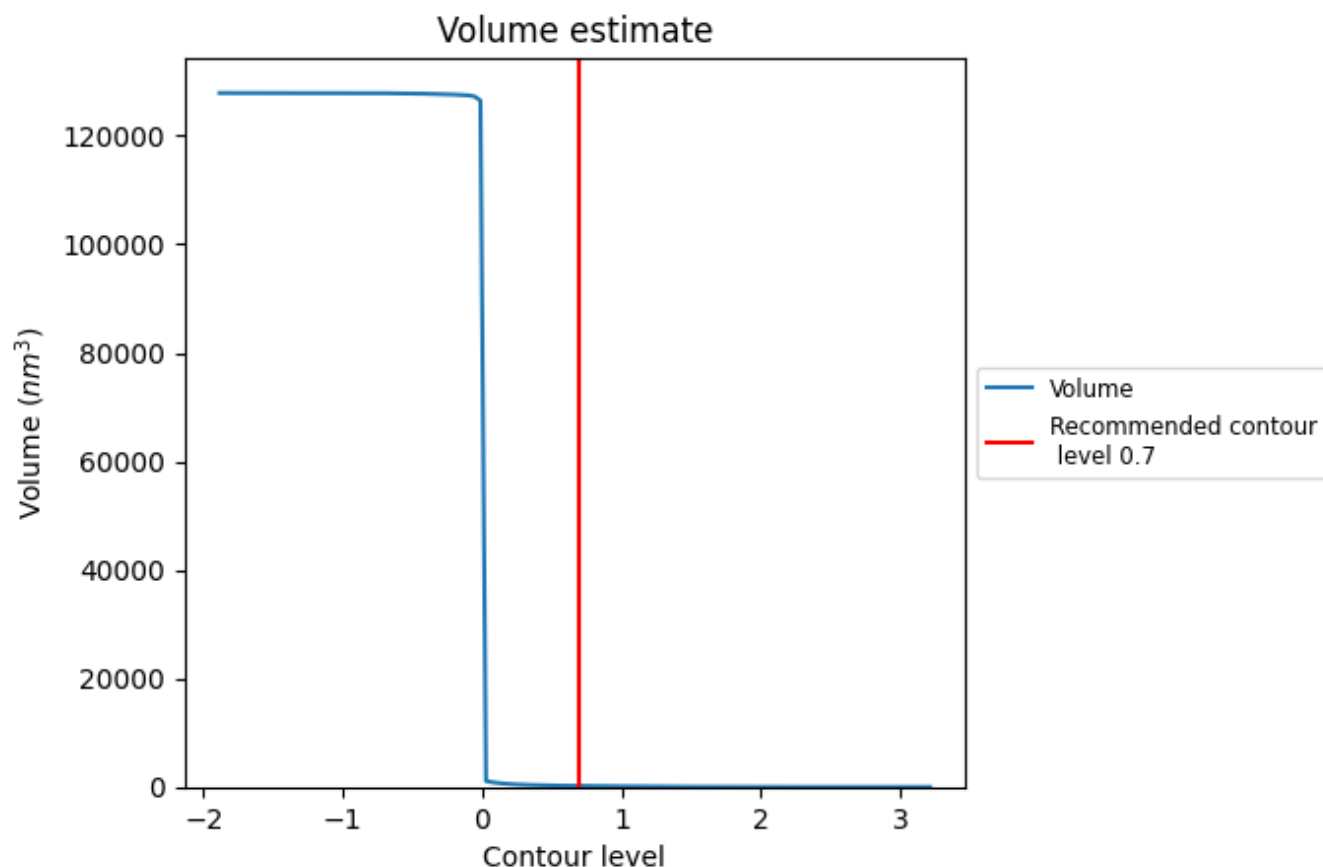
This section contains the results of statistical analysis of the map.

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



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

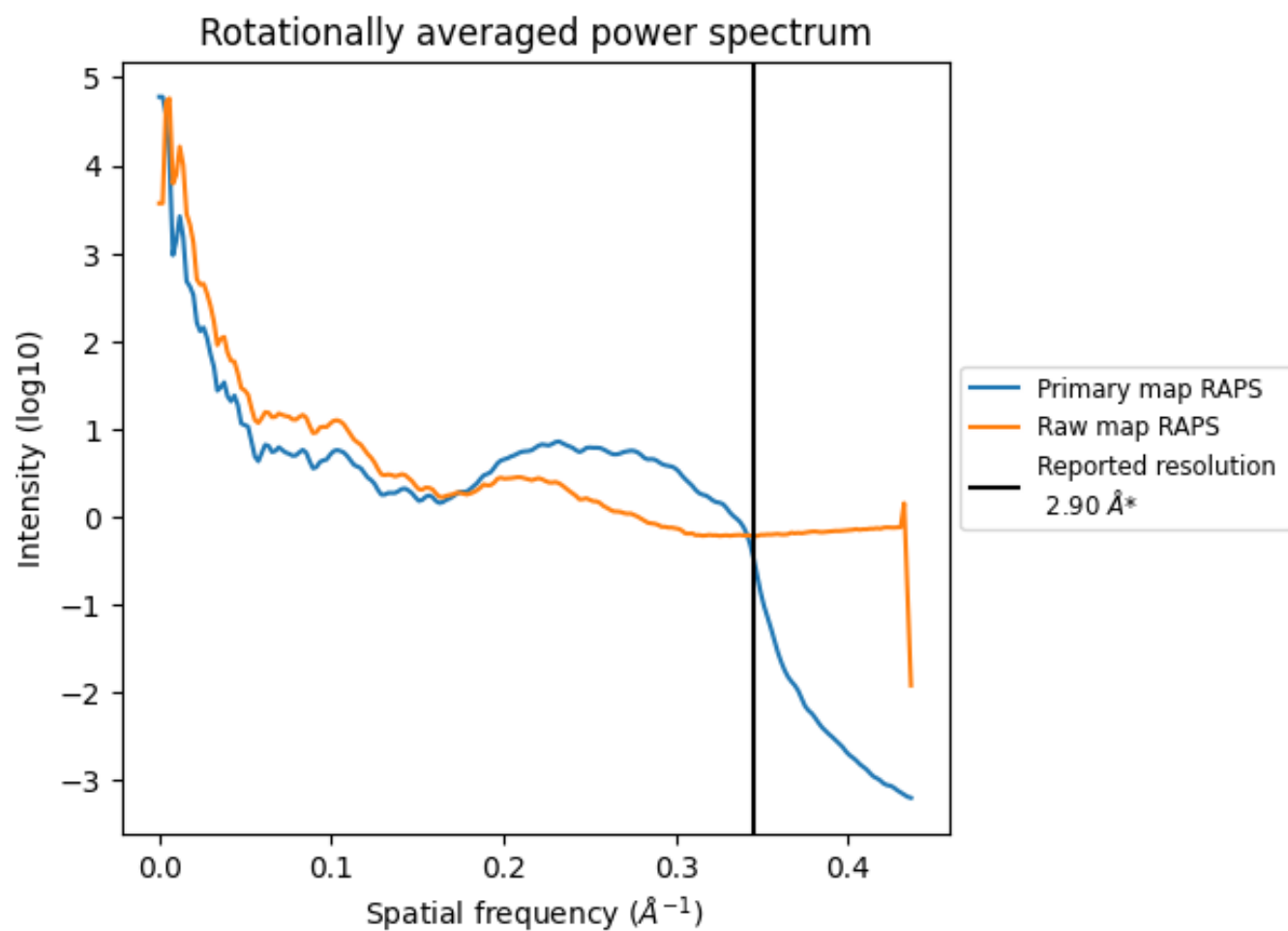
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 188 nm<sup>3</sup>; this corresponds to an approximate mass of 170 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 ⓘ

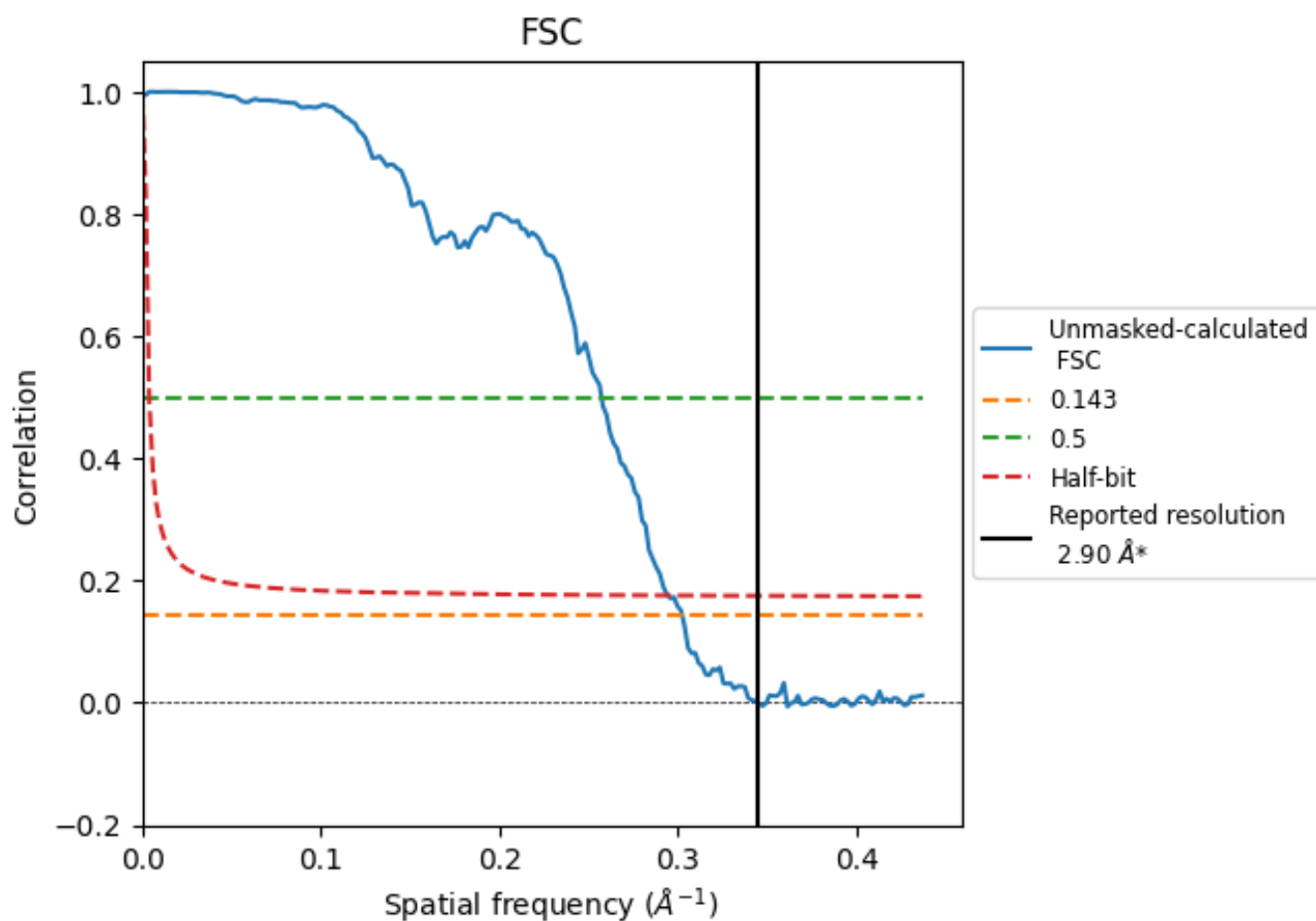


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.345  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

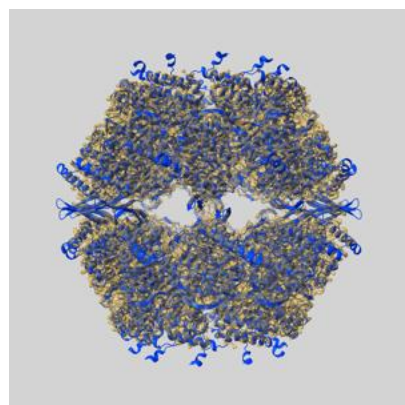
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.90                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.31                               | 3.89 | 3.40     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.31 differs from the reported value 2.9 by more than 10 %

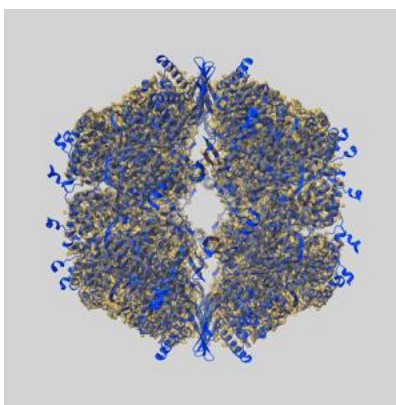
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17031 and PDB model 8OOU. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

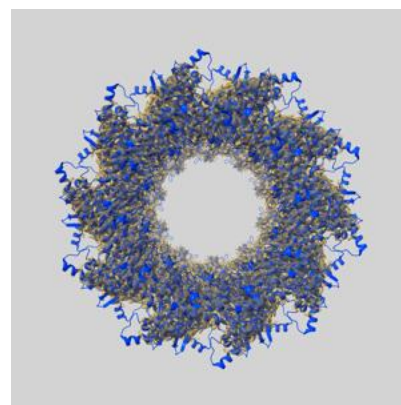
### 9.1 Map-model overlay [i](#)



X



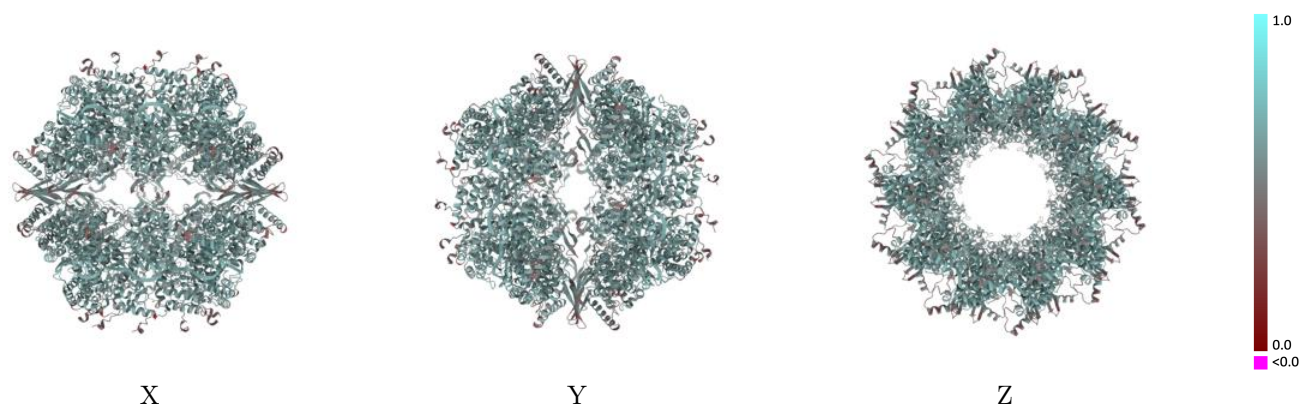
Y



Z

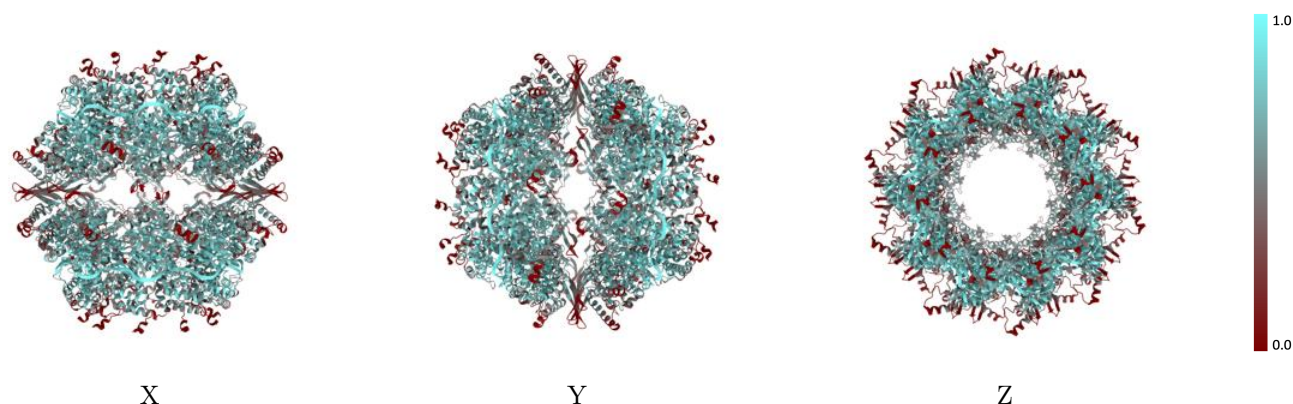
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



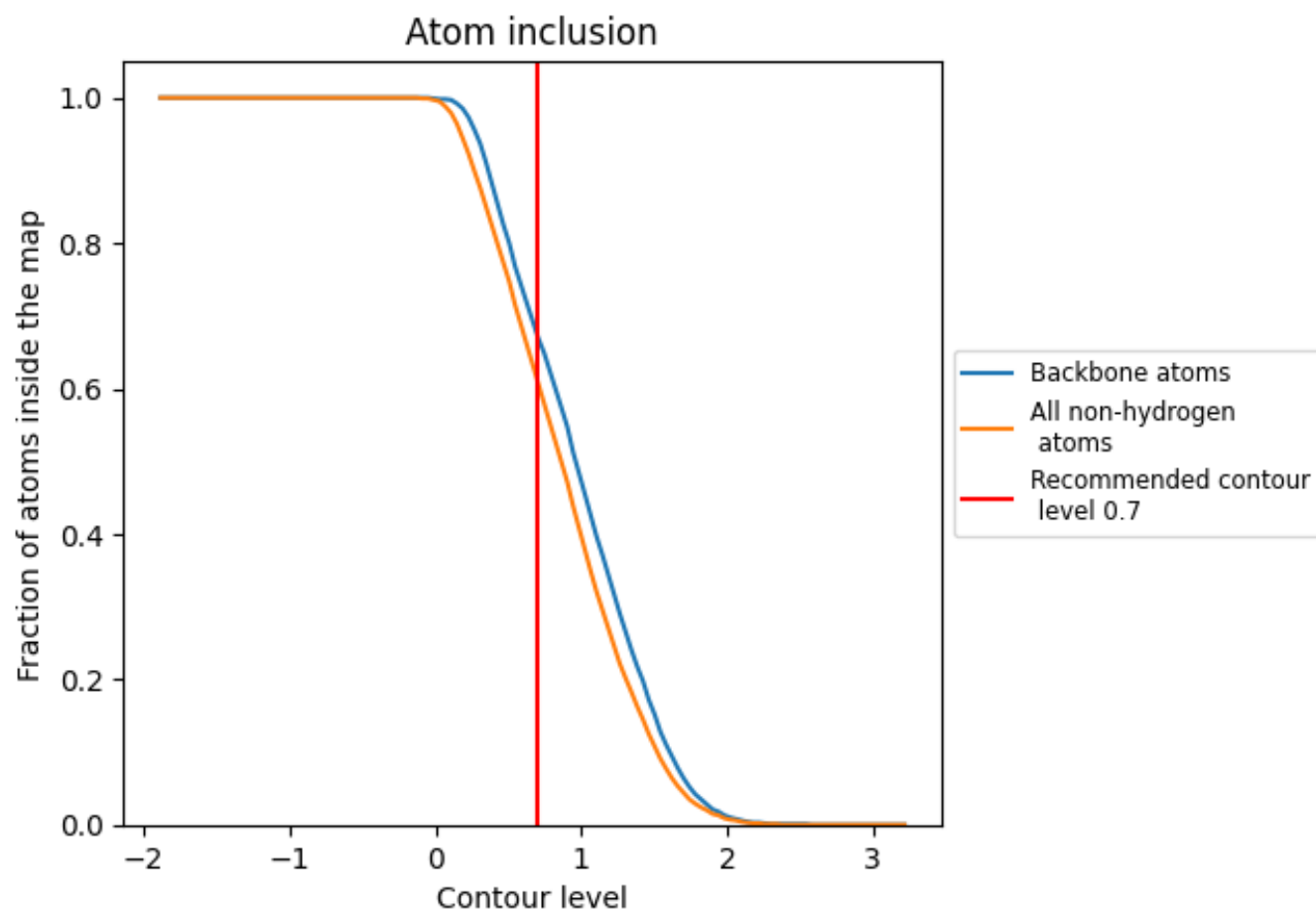
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 67% of all backbone atoms, 61% 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 (0.7) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6110   |  0.5850   |
| A     |  0.5990   |  0.5830   |
| B     |  0.5990   |  0.5820   |
| C     |  0.5980   |  0.5820   |
| D     |  0.5990   |  0.5820   |
| E     |  0.5950   |  0.5820   |
| F     |  0.5990   |  0.5830   |
| G     |  0.5990   |  0.5820   |
| H     |  0.5980   |  0.5820   |
| I     |  0.5990   |  0.5820   |
| J     |  0.5950   |  0.5820   |
| K     |  0.5990   |  0.5840   |
| L     |  0.5990   |  0.5820   |
| M     |  0.5980   |  0.5830   |
| N     |  0.5990  |  0.5820  |
| O     |  0.5950 |  0.5830 |
| P     |  0.5990 |  0.5830 |
| Q     |  0.5990 |  0.5820 |
| R     |  0.5980 |  0.5820 |
| S     |  0.5990 |  0.5820 |
| T     |  0.5950 |  0.5820 |
| U     |  0.8830 |  0.6270 |
| e     |  0.8830 |  0.6270 |

