



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:44 AM UTC

PDB ID : 8UBE / pdb\_00008ube  
EMDB ID : EMD-42084  
Title : Diversity-generating retroelement (DGR) ribonucleoprotein reverse transcriptase - Resting State 1a  
Authors : Biswas, T.; Handa, S.; Ghosh, P.  
Deposited on : 2023-09-22  
Resolution : 3.05 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

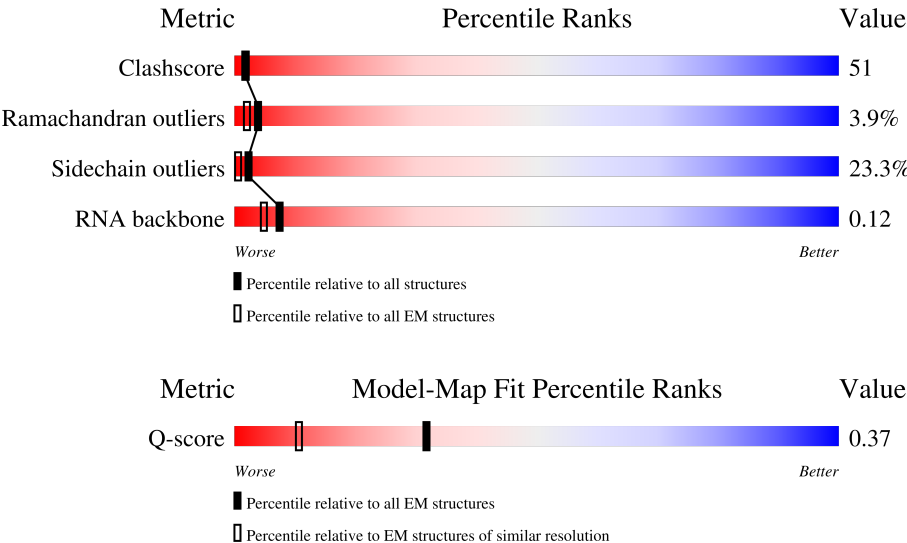
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.05 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                       | 13971 ( 2.55 - 3.55 )                                    |

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     | 328    |                  |
| 2   | B     | 290    |                  |
| 2   | C     | 290    |                  |

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| Mol | Chain | Length | Quality of chain                                                                  |
|-----|-------|--------|-----------------------------------------------------------------------------------|
| 2   | D     | 290    | <div><div><div></div><div></div><div></div></div><div>9%26%62%</div></div>        |
| 2   | E     | 290    | <div><div><div></div><div></div><div></div></div><div>10%23%62%</div></div>       |
| 2   | F     | 290    | <div><div><div></div><div></div><div></div></div><div>11%21%5%62%</div></div>     |
| 3   | G     | 19     | <div><div><div></div><div></div><div></div></div><div>16%37%32%11%42%</div></div> |
| 4   | H     | 36     | <div><div><div></div><div></div><div></div></div><div>6%28%33%8%53%</div></div>   |
| 5   | I     | 140    | <div><div><div></div><div></div><div></div></div><div>14%31%39%34%12%</div></div> |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10613 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 Reverse transcriptase.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 313      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2562  | 1638 | 473 | 442 | 9 |         |       |

- Molecule 2 is a protein called Avd.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | B     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 976   | 631 | 172 | 166 | 7 |         |       |
| 2   | C     | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 888   | 578 | 157 | 148 | 5 |         |       |
| 2   | D     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 879   | 571 | 159 | 144 | 5 |         |       |
| 2   | E     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 569 | 156 | 146 | 5 |         |       |
| 2   | F     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 879   | 571 | 159 | 144 | 5 |         |       |

- Molecule 3 is a RNA chain called Diversity-generating retroelement (DGR) RNA avd.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 3   | G     | 11       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 243   | 107 | 48 | 77 | 11 |         |       |

- Molecule 4 is a RNA chain called Diversity-generating retroelement (DGR) RNA TR.

| Mol | Chain | Residues | Atoms |     |    |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|-------|
| 4   | H     | 17       | Total | C   | N  | O   | P  | 0       | 0     |
|     |       |          | 350   | 157 | 53 | 123 | 17 |         |       |

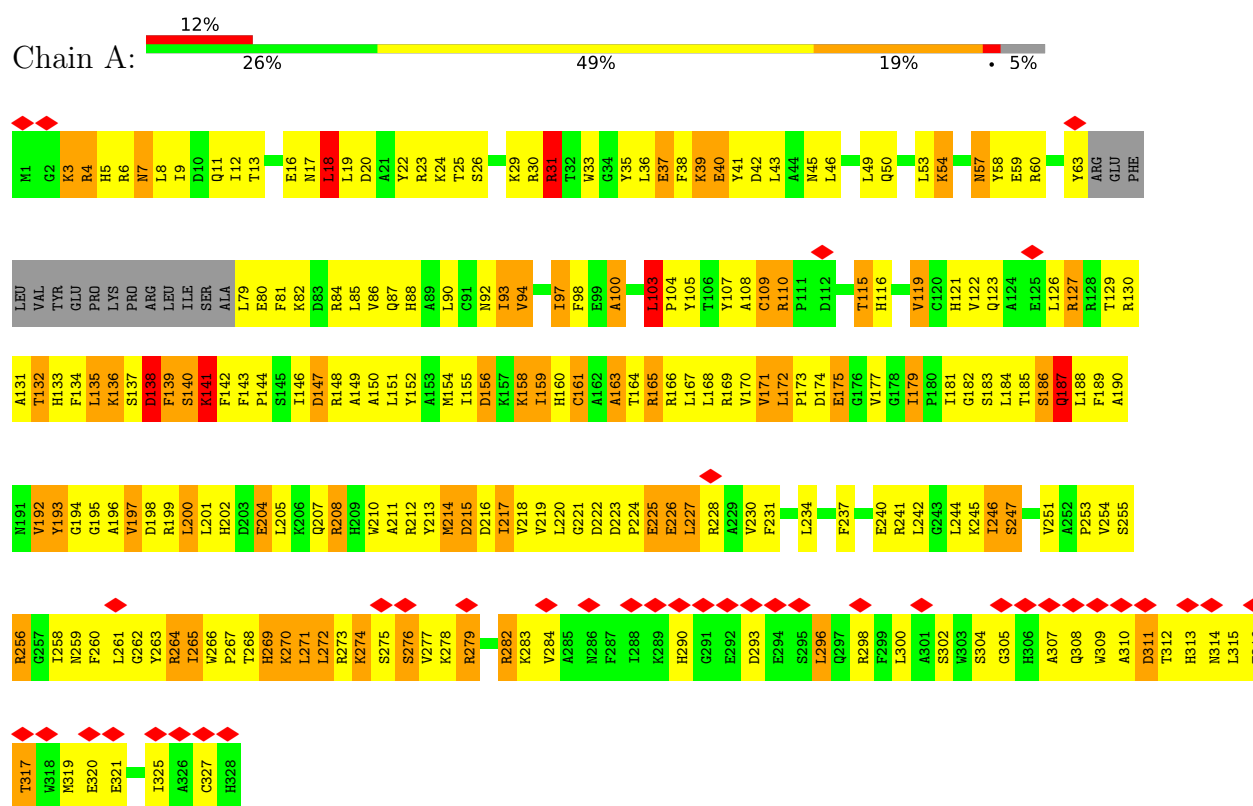
- Molecule 5 is a RNA chain called Diversity-generating retroelement (DGR) RNA Sp.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 5   | I     | 139      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2960  | 1320 | 523 | 978 | 139 |         |       |

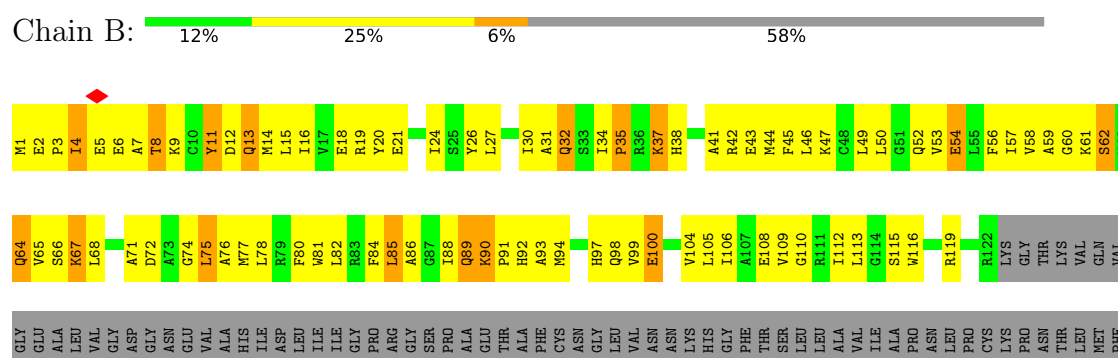
### 3 Residue-property plots

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.

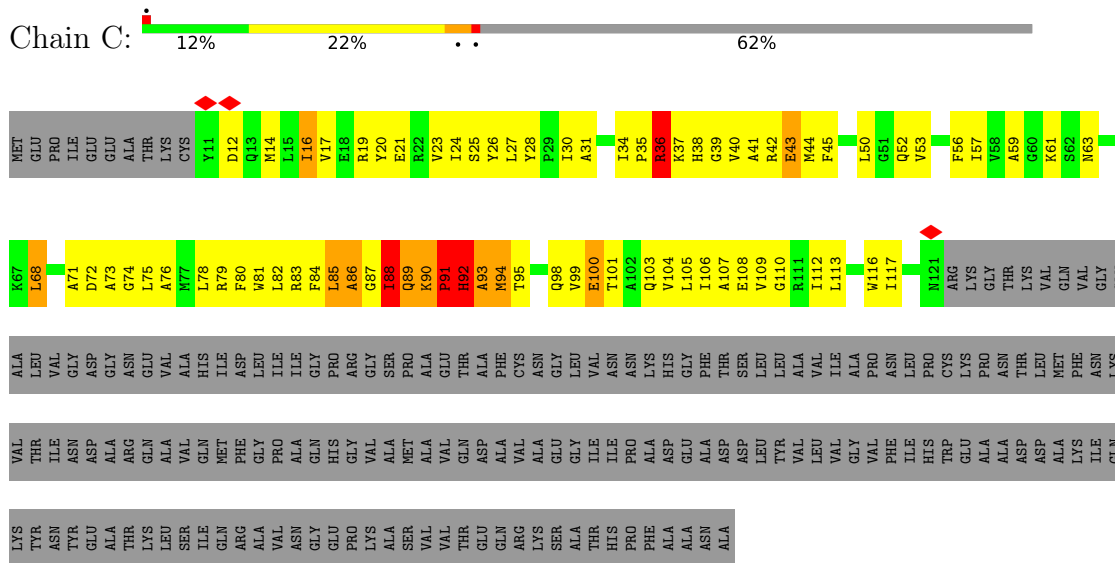
#### • Molecule 1: Reverse transcriptase



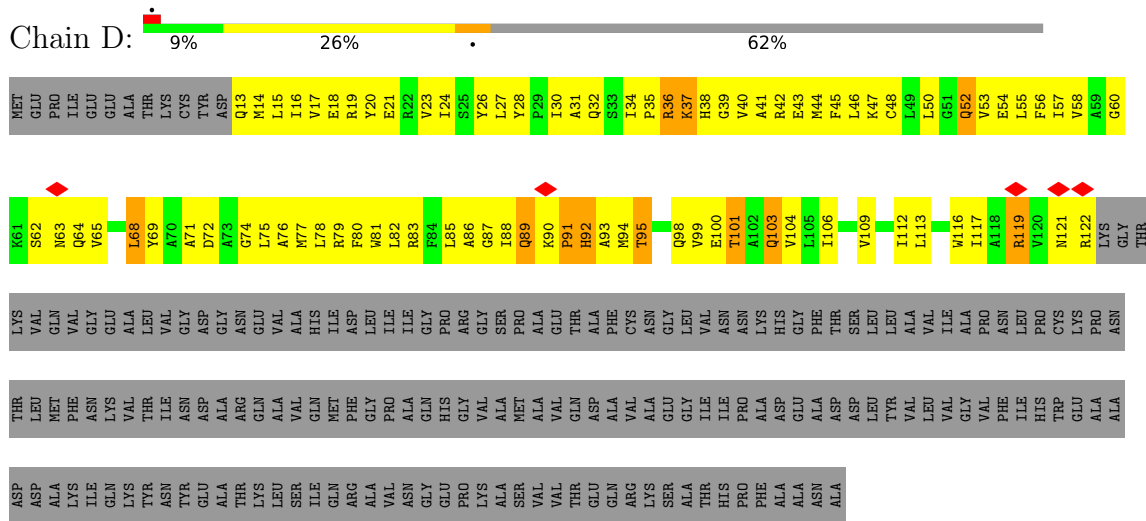
#### • Molecule 2: Avd



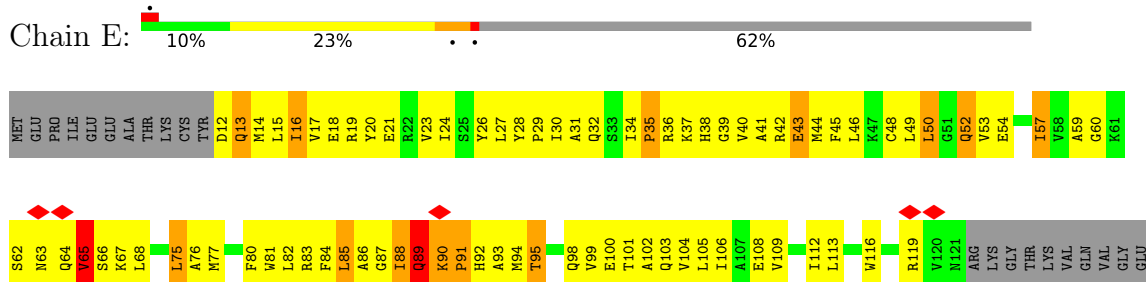
- Molecule 2: Avd



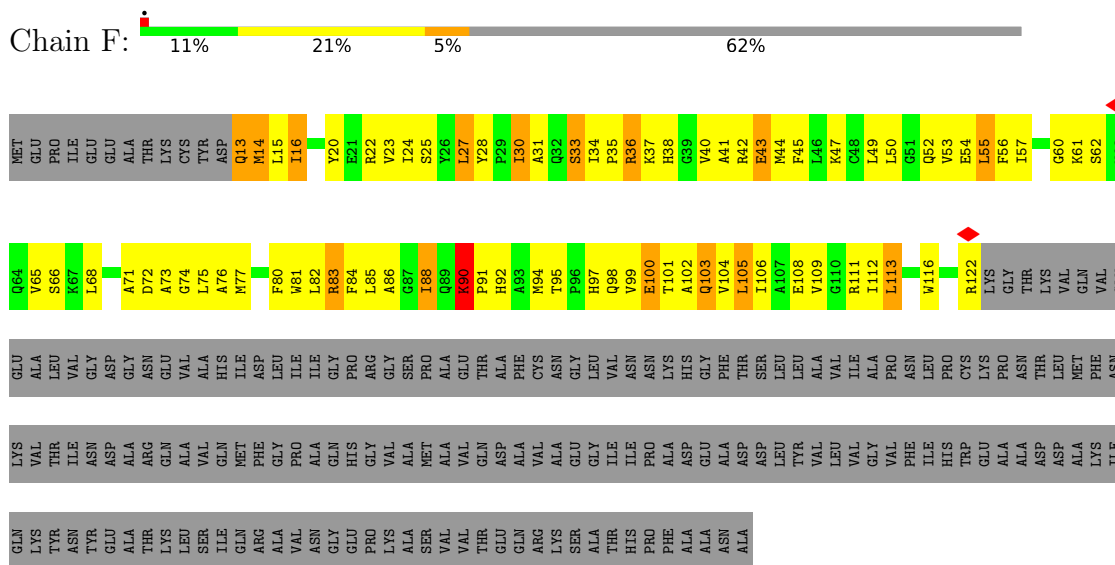
- Molecule 2: Avd



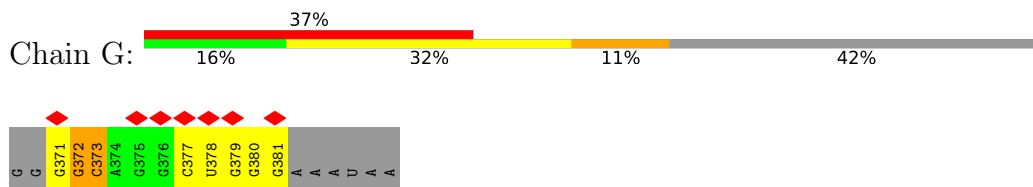
- Molecule 2: Avd



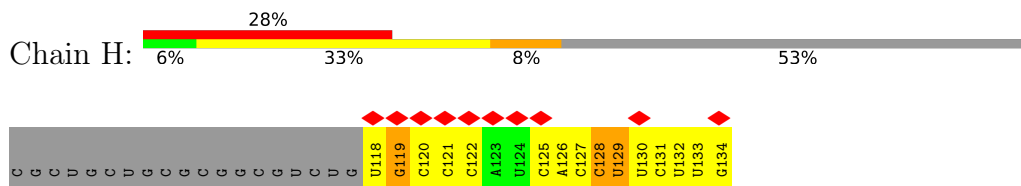
- Molecule 2: Avd



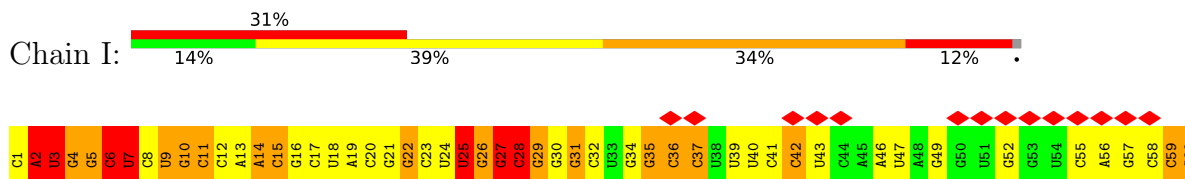
- Molecule 3: Diversity-generating retroelement (DGR) RNA and



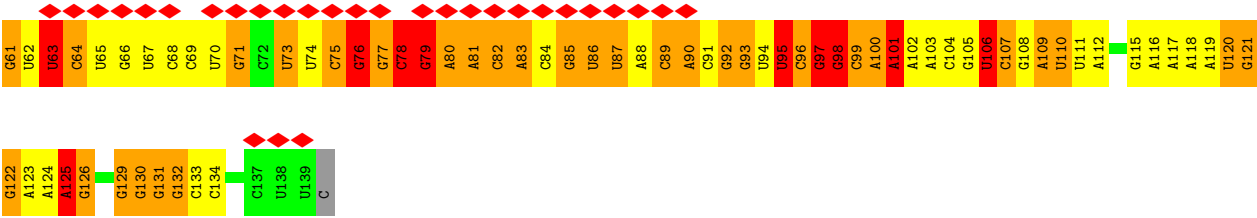
- Molecule 4: Diversity-generating retroelement (DGR) RNA TR



- Molecule 5: Diversity-generating retroelement (DGR) RNA Sp







## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE     | Depositor |
| Imposed symmetry                     | POINT, Not provided |           |
| Number of particles used             | 189678              | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF   | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY | Depositor |
| Microscope                           | FEI TITAN KRIOS     | Depositor |
| Voltage (kV)                         | 300                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 55                  | Depositor |
| Minimum defocus (nm)                 | 400                 | Depositor |
| Maximum defocus (nm)                 | 2000                | Depositor |
| Magnification                        | Not provided        |           |
| Image detector                       | GATAN K3 (6k x 4k)  | Depositor |
| Maximum map value                    | 2.009               | Depositor |
| Minimum map value                    | -1.325              | Depositor |
| Average map value                    | -0.000              | Depositor |
| Map value standard deviation         | 0.030               | Depositor |
| Recommended contour level            | 0.2                 | Depositor |
| Map size ( $\text{\AA}$ )            | 320.0, 320.0, 320.0 | wwPDB     |
| Map dimensions                       | 320, 320, 320       | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0    | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.0, 1.0, 1.0       | 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     | 0.71         | 0/2628         | 1.13        | 8/3549 (0.2%)   |
| 2   | B     | 0.75         | 0/996          | 0.99        | 1/1345 (0.1%)   |
| 2   | C     | 0.79         | 0/907          | 1.10        | 4/1226 (0.3%)   |
| 2   | D     | 0.71         | 0/897          | 0.91        | 1/1211 (0.1%)   |
| 2   | E     | 0.78         | 1/894 (0.1%)   | 0.97        | 0/1208          |
| 2   | F     | 0.76         | 0/897          | 0.99        | 0/1211          |
| 3   | G     | 0.57         | 0/272          | 0.74        | 0/424           |
| 4   | H     | 0.63         | 0/387          | 0.82        | 0/598           |
| 5   | I     | 0.63         | 0/3306         | 1.04        | 24/5151 (0.5%)  |
| All | All   | 0.70         | 1/11184 (0.0%) | 1.03        | 38/15923 (0.2%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | E     | 35  | PRO  | C-O   | -5.53 | 1.17        | 1.23     |

All (38) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 5   | I     | 28  | C    | P-O3'-C3'   | -10.35 | 104.67      | 120.20   |
| 5   | I     | 106 | U    | P-O3'-C3'   | -10.04 | 105.15      | 120.20   |
| 5   | I     | 107 | C    | P-O3'-C3'   | -9.46  | 106.00      | 120.20   |
| 5   | I     | 26  | G    | P-O3'-C3'   | -8.84  | 106.94      | 120.20   |
| 5   | I     | 78  | C    | P-O3'-C3'   | -8.79  | 107.01      | 120.20   |
| 5   | I     | 76  | G    | P-O3'-C3'   | -8.74  | 107.08      | 120.20   |
| 2   | C     | 91  | PRO  | N-CA-CB     | -8.59  | 94.23       | 103.25   |
| 5   | I     | 27  | G    | P-O3'-C3'   | -8.02  | 108.17      | 120.20   |
| 5   | I     | 7   | U    | P-O3'-C3'   | -7.43  | 109.06      | 120.20   |
| 5   | I     | 79  | G    | P-O3'-C3'   | -7.37  | 109.15      | 120.20   |
| 5   | I     | 3   | U    | C2'-C3'-O3' | -6.90  | 103.35      | 113.70   |
| 1   | A     | 311 | ASP  | CA-CB-CG    | -6.88  | 105.72      | 112.60   |
| 5   | I     | 2   | A    | P-O3'-C3'   | -6.86  | 109.92      | 120.20   |
| 5   | I     | 25  | U    | P-O3'-C3'   | -6.47  | 110.50      | 120.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | I     | 125 | A    | P-O3'-C3'   | -5.92 | 111.33      | 120.20   |
| 1   | A     | 311 | ASP  | CA-C-N      | -5.82 | 113.86      | 122.83   |
| 1   | A     | 311 | ASP  | C-N-CA      | -5.82 | 113.86      | 122.83   |
| 5   | I     | 6   | C    | P-O3'-C3'   | -5.74 | 111.59      | 120.20   |
| 2   | B     | 11  | TYR  | CB-CA-C     | -5.69 | 101.94      | 110.88   |
| 5   | I     | 101 | A    | P-O3'-C3'   | -5.67 | 111.70      | 120.20   |
| 5   | I     | 98  | G    | P-O3'-C3'   | -5.65 | 111.72      | 120.20   |
| 5   | I     | 122 | G    | P-O3'-C3'   | -5.63 | 111.76      | 120.20   |
| 2   | C     | 86  | ALA  | N-CA-C      | -5.60 | 98.87       | 110.80   |
| 5   | I     | 95  | U    | P-O3'-C3'   | -5.57 | 111.84      | 120.20   |
| 1   | A     | 31  | ARG  | N-CA-C      | -5.54 | 104.29      | 111.71   |
| 5   | I     | 10  | G    | P-O3'-C3'   | -5.47 | 112.00      | 120.20   |
| 2   | C     | 36  | ARG  | N-CA-C      | -5.41 | 105.38      | 111.28   |
| 1   | A     | 18  | LEU  | N-CA-C      | -5.41 | 106.52      | 113.01   |
| 5   | I     | 63  | U    | C2'-C3'-O3' | 5.34  | 121.72      | 113.70   |
| 5   | I     | 97  | G    | P-O3'-C3'   | -5.34 | 112.19      | 120.20   |
| 5   | I     | 96  | C    | P-O3'-C3'   | -5.28 | 112.29      | 120.20   |
| 2   | C     | 100 | GLU  | N-CA-C      | -5.27 | 105.23      | 110.97   |
| 2   | D     | 91  | PRO  | N-CA-C      | -5.24 | 101.67      | 112.47   |
| 1   | A     | 100 | ALA  | N-CA-C      | -5.15 | 107.12      | 113.41   |
| 1   | A     | 192 | VAL  | N-CA-C      | -5.10 | 106.68      | 111.48   |
| 1   | A     | 183 | SER  | N-CA-C      | -5.07 | 100.08      | 108.75   |
| 5   | I     | 121 | G    | P-O3'-C3'   | -5.03 | 112.66      | 120.20   |
| 5   | I     | 4   | G    | P-O3'-C3'   | -5.01 | 112.69      | 120.20   |

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     | 2562  | 0        | 2550     | 390     | 0            |
| 2   | B     | 976   | 0        | 1014     | 137     | 0            |
| 2   | C     | 888   | 0        | 923      | 129     | 0            |
| 2   | D     | 879   | 0        | 923      | 119     | 0            |
| 2   | E     | 876   | 0        | 914      | 117     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | F     | 879   | 0        | 923      | 95      | 0            |
| 3   | G     | 243   | 0        | 121      | 5       | 0            |
| 4   | H     | 350   | 0        | 181      | 4       | 0            |
| 5   | I     | 2960  | 0        | 1498     | 144     | 0            |
| All | All   | 10613 | 0        | 9047     | 985     | 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 51.

All (985) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:13:GLN:HB3   | 2:E:60:GLY:HA3   | 1.35                     | 1.06              |
| 1:A:163:ALA:HB2  | 5:I:120:U:O4     | 1.57                     | 1.02              |
| 1:A:115:THR:HG23 | 1:A:261:LEU:HD22 | 1.41                     | 1.02              |
| 1:A:141:LYS:HA   | 1:A:308:GLN:HB2  | 1.41                     | 1.02              |
| 1:A:196:ALA:HB3  | 1:A:242:LEU:HD11 | 1.46                     | 0.98              |
| 1:A:18:LEU:HD11  | 1:A:53:LEU:HD12  | 1.42                     | 0.97              |
| 2:D:75:LEU:HD22  | 2:D:106:ILE:HG23 | 1.46                     | 0.97              |
| 1:A:213:TYR:CG   | 1:A:261:LEU:HD21 | 2.00                     | 0.96              |
| 2:E:86:ALA:HB2   | 2:E:99:VAL:HG21  | 1.45                     | 0.95              |
| 2:F:82:LEU:HD11  | 2:F:106:ILE:HD12 | 1.47                     | 0.95              |
| 2:C:82:LEU:HD11  | 2:C:106:ILE:HD12 | 1.49                     | 0.94              |
| 1:A:216:ASP:H    | 1:A:311:ASP:CG   | 1.79                     | 0.91              |
| 1:A:168:LEU:HD22 | 1:A:189:PHE:HZ   | 1.36                     | 0.90              |
| 2:C:50:LEU:O     | 2:D:77:MET:HE1   | 1.71                     | 0.90              |
| 2:E:53:VAL:HG11  | 2:F:80:PHE:CG    | 2.07                     | 0.88              |
| 1:A:274:LYS:HD2  | 1:A:278:LYS:NZ   | 1.88                     | 0.87              |
| 1:A:305:GLY:HA2  | 1:A:308:GLN:OE1  | 1.74                     | 0.87              |
| 2:B:13:GLN:NE2   | 2:B:61:LYS:HD3   | 1.88                     | 0.87              |
| 1:A:140:SER:HA   | 1:A:309:TRP:CE3  | 2.09                     | 0.86              |
| 1:A:182:GLY:HA3  | 1:A:320:GLU:OE1  | 1.76                     | 0.86              |
| 2:B:77:MET:HE1   | 2:F:50:LEU:O     | 1.74                     | 0.85              |
| 2:E:53:VAL:HG11  | 2:F:80:PHE:CD1   | 2.11                     | 0.85              |
| 1:A:11:GLN:HB2   | 1:A:93:ILE:HG12  | 1.58                     | 0.84              |
| 1:A:274:LYS:HD2  | 1:A:278:LYS:HZ3  | 1.43                     | 0.84              |
| 1:A:200:LEU:HD13 | 1:A:237:PHE:CD1  | 2.13                     | 0.83              |
| 2:C:82:LEU:HB3   | 2:C:99:VAL:HG13  | 1.61                     | 0.83              |
| 2:F:75:LEU:HD12  | 2:F:113:LEU:HD12 | 1.61                     | 0.83              |
| 2:B:34:ILE:HD11  | 2:B:85:LEU:HD13  | 1.59                     | 0.82              |
| 2:D:82:LEU:HD11  | 2:D:106:ILE:HD12 | 1.60                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:146:ILE:HG12 | 1:A:193:TYR:HD2  | 1.44                     | 0.81              |
| 2:D:24:ILE:HD11  | 2:D:53:VAL:CG2   | 2.09                     | 0.81              |
| 2:B:61:LYS:HG3   | 2:C:73:ALA:HA    | 1.63                     | 0.81              |
| 2:C:38:HIS:CE1   | 2:C:90:LYS:HD2   | 2.16                     | 0.81              |
| 2:F:82:LEU:HB3   | 2:F:99:VAL:HG13  | 1.63                     | 0.81              |
| 1:A:13:THR:HA    | 1:A:18:LEU:HD12  | 1.64                     | 0.80              |
| 1:A:139:PHE:CZ   | 1:A:197:VAL:HG11 | 2.16                     | 0.80              |
| 1:A:168:LEU:HD22 | 1:A:189:PHE:CZ   | 2.15                     | 0.80              |
| 2:E:75:LEU:HD21  | 2:E:109:VAL:HG23 | 1.64                     | 0.80              |
| 2:B:13:GLN:HE21  | 2:B:61:LYS:HD3   | 1.47                     | 0.79              |
| 2:B:68:LEU:HD21  | 2:B:116:TRP:CE2  | 2.17                     | 0.79              |
| 1:A:151:LEU:HD13 | 1:A:193:TYR:HB2  | 1.63                     | 0.79              |
| 2:B:88:ILE:HG23  | 2:F:25:SER:HA    | 1.64                     | 0.78              |
| 2:C:59:ALA:HB1   | 2:C:68:LEU:HD23  | 1.64                     | 0.78              |
| 5:I:22:G:H2'     | 5:I:23:C:O4'     | 1.84                     | 0.78              |
| 1:A:212:ARG:HB2  | 1:A:217:ILE:HG23 | 1.65                     | 0.78              |
| 1:A:213:TYR:CD2  | 1:A:261:LEU:HD21 | 2.18                     | 0.78              |
| 1:A:104:PRO:HG3  | 5:I:130:G:H4'    | 1.66                     | 0.77              |
| 2:D:43:GLU:HG2   | 2:E:40:VAL:HG22  | 1.65                     | 0.77              |
| 2:D:50:LEU:O     | 2:E:77:MET:HE1   | 1.84                     | 0.77              |
| 1:A:256:ARG:HH12 | 5:I:78:C:H41     | 1.31                     | 0.77              |
| 2:C:85:LEU:HB3   | 2:C:93:ALA:HB3   | 1.67                     | 0.77              |
| 1:A:221:GLY:HA3  | 1:A:227:LEU:HD21 | 1.65                     | 0.77              |
| 2:E:95:THR:HG21  | 5:I:18:U:H4'     | 1.66                     | 0.77              |
| 5:I:101:A:H62    | 5:I:132:G:H21    | 1.31                     | 0.76              |
| 2:F:27:LEU:HG    | 2:F:45:PHE:HZ    | 1.51                     | 0.76              |
| 5:I:124:A:H2'    | 5:I:125:A:H8     | 1.51                     | 0.76              |
| 2:C:57:ILE:HG21  | 2:D:76:ALA:HB3   | 1.68                     | 0.76              |
| 1:A:29:LYS:HE3   | 1:A:321:GLU:HA   | 1.67                     | 0.75              |
| 1:A:94:VAL:HG12  | 1:A:188:LEU:HD21 | 1.66                     | 0.75              |
| 2:C:25:SER:HA    | 2:D:88:ILE:HG23  | 1.68                     | 0.75              |
| 5:I:25:U:H2'     | 5:I:26:G:H8      | 1.52                     | 0.75              |
| 2:D:86:ALA:HB2   | 2:D:99:VAL:HG21  | 1.69                     | 0.75              |
| 1:A:219:VAL:HG11 | 1:A:230:VAL:HG11 | 1.67                     | 0.74              |
| 2:B:21:GLU:OE2   | 2:C:83:ARG:HD2   | 1.86                     | 0.74              |
| 2:E:86:ALA:HB2   | 2:E:99:VAL:CG2   | 2.17                     | 0.74              |
| 2:E:34:ILE:HD13  | 2:E:85:LEU:HG    | 1.68                     | 0.74              |
| 2:C:41:ALA:HB1   | 2:C:84:PHE:HE2   | 1.52                     | 0.74              |
| 1:A:265:ILE:HG23 | 1:A:270:LYS:HB3  | 1.70                     | 0.73              |
| 2:E:53:VAL:HG21  | 2:F:80:PHE:CZ    | 2.23                     | 0.73              |
| 2:E:86:ALA:CB    | 2:E:99:VAL:HG21  | 2.18                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:82:LEU:HD11  | 2:C:106:ILE:CD1  | 2.18                     | 0.73              |
| 2:F:97:HIS:O     | 2:F:101:THR:N    | 2.20                     | 0.73              |
| 1:A:39:LYS:HA    | 1:A:42:ASP:HB3   | 1.69                     | 0.73              |
| 1:A:141:LYS:CA   | 1:A:308:GLN:HB2  | 2.19                     | 0.72              |
| 2:B:86:ALA:HB2   | 2:B:99:VAL:HG21  | 1.69                     | 0.72              |
| 2:E:82:LEU:HB3   | 2:E:99:VAL:HG13  | 1.72                     | 0.72              |
| 2:B:56:PHE:O     | 2:B:60:GLY:N     | 2.22                     | 0.72              |
| 1:A:4:ARG:O      | 1:A:160:HIS:HB2  | 1.89                     | 0.72              |
| 2:D:45:PHE:CD2   | 2:D:85:LEU:HD11  | 2.25                     | 0.72              |
| 2:B:61:LYS:NZ    | 2:C:76:ALA:HB2   | 2.05                     | 0.72              |
| 2:B:15:LEU:HG    | 2:B:112:ILE:HD13 | 1.70                     | 0.71              |
| 2:B:45:PHE:CD2   | 2:B:85:LEU:HD11  | 2.25                     | 0.71              |
| 2:B:84:PHE:CD2   | 2:B:85:LEU:HD23  | 2.26                     | 0.71              |
| 1:A:140:SER:HA   | 1:A:309:TRP:CZ3  | 2.26                     | 0.71              |
| 2:C:89:GLN:HG3   | 2:C:90:LYS:HG3   | 1.71                     | 0.71              |
| 5:I:27:G:H3'     | 5:I:28:C:H6      | 1.55                     | 0.71              |
| 1:A:313:HIS:O    | 1:A:317:THR:HG23 | 1.90                     | 0.71              |
| 1:A:221:GLY:HA3  | 1:A:227:LEU:HD11 | 1.71                     | 0.71              |
| 2:F:24:ILE:HD11  | 2:F:53:VAL:CG2   | 2.21                     | 0.71              |
| 1:A:105:TYR:O    | 1:A:211:ALA:HA   | 1.90                     | 0.70              |
| 2:B:21:GLU:CD    | 2:C:83:ARG:HH11  | 1.99                     | 0.70              |
| 2:B:84:PHE:HD2   | 2:B:85:LEU:HD23  | 1.56                     | 0.70              |
| 5:I:124:A:H2'    | 5:I:125:A:C8     | 2.26                     | 0.70              |
| 1:A:126:LEU:HD22 | 1:A:254:VAL:HG11 | 1.72                     | 0.70              |
| 1:A:6:ARG:NH1    | 5:I:122:G:N7     | 2.40                     | 0.70              |
| 1:A:80:GLU:O     | 1:A:84:ARG:HG3   | 1.92                     | 0.70              |
| 1:A:108:ALA:HB2  | 1:A:213:TYR:C    | 2.17                     | 0.70              |
| 2:D:54:GLU:OE1   | 2:E:77:MET:HB2   | 1.92                     | 0.70              |
| 2:D:38:HIS:NE2   | 2:D:91:PRO:HD2   | 2.07                     | 0.70              |
| 1:A:163:ALA:CB   | 5:I:120:U:O4     | 2.39                     | 0.70              |
| 2:C:82:LEU:HD22  | 2:C:94:MET:SD    | 2.32                     | 0.70              |
| 2:E:59:ALA:C     | 2:E:116:TRP:HH2  | 2.00                     | 0.70              |
| 1:A:136:LYS:HE2  | 1:A:216:ASP:HB2  | 1.72                     | 0.69              |
| 2:C:40:VAL:HG23  | 5:I:3:U:O4       | 1.92                     | 0.69              |
| 1:A:103:LEU:HD23 | 1:A:104:PRO:HD2  | 1.72                     | 0.69              |
| 1:A:217:ILE:O    | 1:A:219:VAL:HG23 | 1.91                     | 0.69              |
| 2:D:86:ALA:CB    | 2:D:99:VAL:HG21  | 2.22                     | 0.69              |
| 2:C:53:VAL:HG11  | 2:D:80:PHE:CD1   | 2.27                     | 0.69              |
| 1:A:143:PHE:HZ   | 1:A:214:MET:HE3  | 1.56                     | 0.69              |
| 2:B:81:TRP:HH2   | 2:F:50:LEU:HD13  | 1.57                     | 0.69              |
| 5:I:5:G:H5''     | 5:I:5:G:H8       | 1.58                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:208:ARG:HG2  | 5:I:130:G:OP1    | 1.93                     | 0.68              |
| 2:E:35:PRO:HD3   | 2:E:93:ALA:HA    | 1.76                     | 0.68              |
| 1:A:36:LEU:HB3   | 2:B:14:MET:HB3   | 1.74                     | 0.68              |
| 1:A:133:HIS:CD2  | 1:A:253:PRO:HB3  | 2.27                     | 0.68              |
| 1:A:146:ILE:HG23 | 1:A:193:TYR:CD2  | 2.28                     | 0.68              |
| 2:E:98:GLN:NE2   | 5:I:17:C:O3'     | 2.26                     | 0.68              |
| 1:A:213:TYR:CD1  | 1:A:261:LEU:HD11 | 2.29                     | 0.68              |
| 1:A:41:TYR:CE2   | 2:C:107:ALA:HA   | 2.29                     | 0.68              |
| 1:A:134:PHE:CE1  | 1:A:258:ILE:HG12 | 2.28                     | 0.68              |
| 2:C:38:HIS:HE1   | 2:C:90:LYS:HD2   | 1.59                     | 0.68              |
| 2:E:21:GLU:OE2   | 2:F:83:ARG:HD2   | 1.94                     | 0.68              |
| 1:A:147:ASP:HB2  | 1:A:193:TYR:OH   | 1.94                     | 0.68              |
| 2:B:38:HIS:HA    | 2:F:28:TYR:OH    | 1.92                     | 0.68              |
| 2:E:31:ALA:HA    | 2:E:34:ILE:HG13  | 1.75                     | 0.68              |
| 2:F:23:VAL:HG22  | 2:F:105:LEU:HB3  | 1.76                     | 0.68              |
| 1:A:126:LEU:HG   | 1:A:220:LEU:HD13 | 1.76                     | 0.68              |
| 1:A:223:ASP:HB3  | 1:A:226:GLU:HB2  | 1.76                     | 0.68              |
| 5:I:95:U:H2'     | 5:I:96:C:C6      | 2.28                     | 0.68              |
| 2:C:90:LYS:O     | 2:C:91:PRO:C     | 2.37                     | 0.67              |
| 5:I:25:U:H2'     | 5:I:26:G:C8      | 2.29                     | 0.67              |
| 2:C:92:HIS:H     | 2:C:92:HIS:CD2   | 2.10                     | 0.67              |
| 2:D:30:ILE:HG21  | 2:D:94:MET:HG3   | 1.76                     | 0.67              |
| 2:D:86:ALA:HB2   | 2:D:99:VAL:CG2   | 2.25                     | 0.67              |
| 2:B:34:ILE:HD11  | 2:B:85:LEU:CD1   | 2.25                     | 0.67              |
| 2:C:24:ILE:HG22  | 2:D:88:ILE:HG21  | 1.77                     | 0.67              |
| 2:D:57:ILE:HG21  | 2:E:76:ALA:HB3   | 1.75                     | 0.67              |
| 2:D:52:GLN:HG2   | 2:D:55:LEU:HD12  | 1.75                     | 0.67              |
| 2:B:82:LEU:HB3   | 2:B:99:VAL:HG13  | 1.76                     | 0.67              |
| 1:A:98:PHE:HB2   | 1:A:188:LEU:HD11 | 1.77                     | 0.67              |
| 1:A:53:LEU:HD21  | 1:A:86:VAL:HG22  | 1.76                     | 0.66              |
| 1:A:213:TYR:CD1  | 1:A:261:LEU:HD21 | 2.30                     | 0.66              |
| 2:B:81:TRP:CH2   | 2:F:50:LEU:HD13  | 2.31                     | 0.66              |
| 1:A:213:TYR:O    | 1:A:214:MET:HB2  | 1.96                     | 0.66              |
| 2:E:92:HIS:CE1   | 5:I:19:A:C4      | 2.83                     | 0.66              |
| 1:A:159:ILE:O    | 1:A:160:HIS:HB2  | 1.93                     | 0.66              |
| 2:B:86:ALA:HB2   | 2:B:99:VAL:CG2   | 2.25                     | 0.66              |
| 5:I:108:G:H3'    | 5:I:109:A:H5''   | 1.78                     | 0.66              |
| 2:C:34:ILE:HD13  | 2:C:85:LEU:HD22  | 1.78                     | 0.66              |
| 1:A:38:PHE:HE2   | 2:B:1:MET:HE1    | 1.61                     | 0.66              |
| 1:A:8:LEU:HB2    | 1:A:164:THR:OG1  | 1.96                     | 0.66              |
| 1:A:103:LEU:HD13 | 1:A:202:HIS:HB3  | 1.78                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:92:HIS:O     | 2:C:93:ALA:C     | 2.39                     | 0.66              |
| 1:A:187:GLN:CD   | 1:A:317:THR:HG21 | 2.21                     | 0.65              |
| 5:I:68:C:H2'     | 5:I:69:C:C6      | 2.32                     | 0.65              |
| 2:B:68:LEU:HD21  | 2:B:116:TRP:CZ2  | 2.31                     | 0.65              |
| 2:F:14:MET:CE    | 2:F:60:GLY:HA3   | 2.27                     | 0.65              |
| 1:A:275:SER:O    | 1:A:279:ARG:HB2  | 1.96                     | 0.65              |
| 1:A:272:LEU:HD22 | 5:I:83:A:H61     | 1.60                     | 0.65              |
| 2:B:45:PHE:CD1   | 2:B:81:TRP:HB3   | 2.32                     | 0.65              |
| 2:C:26:TYR:OH    | 2:C:98:GLN:HA    | 1.97                     | 0.65              |
| 2:D:68:LEU:HD11  | 2:D:116:TRP:CE3  | 2.31                     | 0.65              |
| 1:A:172:LEU:HD11 | 1:A:179:ILE:HG12 | 1.79                     | 0.64              |
| 1:A:13:THR:HA    | 1:A:18:LEU:CD1   | 2.27                     | 0.64              |
| 1:A:140:SER:O    | 1:A:142:PHE:N    | 2.31                     | 0.64              |
| 1:A:36:LEU:HD12  | 2:B:11:TYR:CE1   | 2.33                     | 0.64              |
| 1:A:192:VAL:C    | 1:A:194:GLY:H    | 2.03                     | 0.64              |
| 1:A:263:TYR:O    | 1:A:265:ILE:HG13 | 1.98                     | 0.64              |
| 2:D:24:ILE:HD11  | 2:D:53:VAL:HG22  | 1.78                     | 0.64              |
| 1:A:4:ARG:HB3    | 1:A:6:ARG:HG2    | 1.80                     | 0.64              |
| 1:A:12:ILE:HD11  | 1:A:164:THR:HG23 | 1.80                     | 0.64              |
| 1:A:179:ILE:HD13 | 1:A:186:SER:HA   | 1.80                     | 0.64              |
| 2:F:14:MET:HE1   | 2:F:60:GLY:HA3   | 1.80                     | 0.64              |
| 1:A:26:SER:O     | 1:A:30:ARG:HG3   | 1.98                     | 0.63              |
| 1:A:94:VAL:HG12  | 1:A:188:LEU:CD2  | 2.27                     | 0.63              |
| 1:A:187:GLN:HG3  | 1:A:313:HIS:ND1  | 2.12                     | 0.63              |
| 2:F:27:LEU:HD21  | 2:F:82:LEU:HD21  | 1.79                     | 0.63              |
| 2:B:34:ILE:O     | 2:B:42:ARG:NH1   | 2.32                     | 0.63              |
| 2:B:41:ALA:HB2   | 2:F:28:TYR:CE1   | 2.33                     | 0.63              |
| 2:C:24:ILE:HD11  | 2:C:53:VAL:CG2   | 2.28                     | 0.63              |
| 2:C:87:GLY:O     | 2:C:88:ILE:C     | 2.40                     | 0.63              |
| 1:A:228:ARG:HG3  | 1:A:251:VAL:HG21 | 1.81                     | 0.63              |
| 2:C:53:VAL:HG11  | 2:D:80:PHE:CG    | 2.33                     | 0.63              |
| 1:A:147:ASP:HB3  | 1:A:150:ALA:H    | 1.64                     | 0.63              |
| 1:A:103:LEU:HD12 | 1:A:199:ARG:HG2  | 1.80                     | 0.63              |
| 1:A:274:LYS:HB2  | 1:A:278:LYS:HD3  | 1.81                     | 0.63              |
| 2:E:24:ILE:HD11  | 2:E:53:VAL:CG2   | 2.29                     | 0.63              |
| 1:A:107:TYR:OH   | 1:A:121:HIS:HB2  | 1.98                     | 0.62              |
| 1:A:155:ILE:HG22 | 1:A:155:ILE:O    | 1.99                     | 0.62              |
| 5:I:124:A:O2'    | 5:I:125:A:H5'    | 1.98                     | 0.62              |
| 2:F:82:LEU:HD11  | 2:F:106:ILE:CD1  | 2.27                     | 0.62              |
| 1:A:256:ARG:NH2  | 5:I:77:G:N7      | 2.48                     | 0.62              |
| 5:I:29:G:H5''    | 5:I:29:G:H8      | 1.65                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:119:VAL:O    | 1:A:265:ILE:HG21 | 2.00                     | 0.62              |
| 2:B:38:HIS:HA    | 2:F:28:TYR:HH    | 1.64                     | 0.62              |
| 1:A:41:TYR:CD2   | 2:B:4:ILE:HG21   | 2.34                     | 0.62              |
| 1:A:90:LEU:HD13  | 1:A:168:LEU:HD23 | 1.80                     | 0.62              |
| 2:B:27:LEU:HD11  | 2:B:82:LEU:HD21  | 1.82                     | 0.62              |
| 5:I:95:U:H2'     | 5:I:96:C:H6      | 1.65                     | 0.62              |
| 5:I:100:A:H4'    | 5:I:101:A:H8     | 1.65                     | 0.62              |
| 1:A:172:LEU:HD22 | 1:A:189:PHE:HD2  | 1.65                     | 0.62              |
| 1:A:274:LYS:CD   | 1:A:278:LYS:HZ3  | 2.13                     | 0.61              |
| 1:A:313:HIS:O    | 1:A:316:PHE:N    | 2.33                     | 0.61              |
| 2:F:97:HIS:CE1   | 2:F:101:THR:HG21 | 2.35                     | 0.61              |
| 2:F:99:VAL:O     | 2:F:103:GLN:HB2  | 1.99                     | 0.61              |
| 2:B:16:ILE:HD11  | 2:B:113:LEU:HB2  | 1.82                     | 0.61              |
| 5:I:60:G:H2'     | 5:I:61:G:H8      | 1.65                     | 0.61              |
| 1:A:186:SER:O    | 1:A:187:GLN:C    | 2.42                     | 0.61              |
| 1:A:216:ASP:N    | 1:A:311:ASP:OD1  | 2.31                     | 0.61              |
| 2:B:89:GLN:HG2   | 2:B:93:ALA:HB2   | 1.82                     | 0.61              |
| 1:A:276:SER:HA   | 5:I:70:U:H3      | 1.64                     | 0.61              |
| 1:A:172:LEU:HD22 | 1:A:189:PHE:CD2  | 2.36                     | 0.61              |
| 2:C:16:ILE:HD13  | 2:C:112:ILE:HB   | 1.82                     | 0.61              |
| 1:A:98:PHE:CZ    | 1:A:155:ILE:HA   | 2.36                     | 0.61              |
| 2:B:27:LEU:HD23  | 2:B:30:ILE:HD11  | 1.81                     | 0.61              |
| 1:A:202:HIS:NE2  | 5:I:129:G:O2'    | 2.34                     | 0.61              |
| 2:E:52:GLN:OE1   | 2:E:75:LEU:HD13  | 2.01                     | 0.61              |
| 1:A:187:GLN:HG3  | 1:A:313:HIS:HD1  | 1.66                     | 0.61              |
| 1:A:245:LYS:O    | 1:A:309:TRP:CZ3  | 2.54                     | 0.61              |
| 2:E:45:PHE:CD1   | 2:E:81:TRP:HB3   | 2.36                     | 0.61              |
| 1:A:38:PHE:CE2   | 2:B:1:MET:HE1    | 2.35                     | 0.60              |
| 1:A:136:LYS:HD2  | 1:A:218:VAL:HG22 | 1.83                     | 0.60              |
| 1:A:274:LYS:CB   | 1:A:278:LYS:HD3  | 2.31                     | 0.60              |
| 1:A:212:ARG:HG2  | 1:A:214:MET:H    | 1.65                     | 0.60              |
| 2:C:27:LEU:HD11  | 2:C:82:LEU:HD21  | 1.83                     | 0.60              |
| 2:D:68:LEU:HB3   | 2:D:117:ILE:CD1  | 2.32                     | 0.60              |
| 1:A:138:ASP:OD1  | 1:A:216:ASP:HB3  | 2.01                     | 0.60              |
| 1:A:138:ASP:OD2  | 1:A:310:ALA:HA   | 2.01                     | 0.60              |
| 2:C:45:PHE:CD1   | 2:C:81:TRP:HB3   | 2.37                     | 0.60              |
| 1:A:11:GLN:CB    | 1:A:93:ILE:HG12  | 2.28                     | 0.60              |
| 1:A:100:ALA:O    | 5:I:105:G:H4'    | 2.00                     | 0.60              |
| 2:E:23:VAL:CG1   | 2:E:27:LEU:HD12  | 2.32                     | 0.60              |
| 2:B:85:LEU:HD22  | 2:B:89:GLN:NE2   | 2.16                     | 0.60              |
| 1:A:141:LYS:O    | 1:A:142:PHE:C    | 2.44                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:143:PHE:CZ   | 1:A:214:MET:HE3  | 2.36                     | 0.60              |
| 2:D:82:LEU:HD11  | 2:D:106:ILE:CD1  | 2.29                     | 0.60              |
| 1:A:49:LEU:HD23  | 1:A:85:LEU:HD22  | 1.83                     | 0.60              |
| 1:A:105:TYR:CE2  | 1:A:202:HIS:HE1  | 2.20                     | 0.60              |
| 2:E:82:LEU:HD11  | 2:E:106:ILE:HD12 | 1.83                     | 0.60              |
| 1:A:213:TYR:O    | 1:A:311:ASP:HB3  | 2.01                     | 0.59              |
| 1:A:272:LEU:HD22 | 5:I:83:A:N6      | 2.16                     | 0.59              |
| 2:C:52:GLN:OE1   | 2:C:74:GLY:C     | 2.46                     | 0.59              |
| 2:C:90:LYS:HD3   | 5:I:2:A:OP2      | 2.02                     | 0.59              |
| 5:I:102:A:H2'    | 5:I:103:A:C8     | 2.37                     | 0.59              |
| 2:B:82:LEU:HD11  | 2:B:106:ILE:HD12 | 1.83                     | 0.59              |
| 2:D:45:PHE:CD1   | 2:D:81:TRP:HB3   | 2.37                     | 0.59              |
| 1:A:212:ARG:HD2  | 1:A:214:MET:O    | 2.03                     | 0.59              |
| 1:A:221:GLY:CA   | 1:A:227:LEU:HD21 | 2.32                     | 0.59              |
| 2:C:82:LEU:CD1   | 2:C:106:ILE:HD12 | 2.30                     | 0.59              |
| 2:C:100:GLU:O    | 2:C:104:VAL:HG23 | 2.01                     | 0.59              |
| 1:A:199:ARG:NH2  | 5:I:105:G:O2'    | 2.35                     | 0.59              |
| 2:E:36:ARG:O     | 2:E:39:GLY:N     | 2.35                     | 0.59              |
| 2:C:34:ILE:HG22  | 2:C:38:HIS:HB2   | 1.84                     | 0.59              |
| 2:B:68:LEU:HD21  | 2:B:116:TRP:CD2  | 2.37                     | 0.59              |
| 5:I:27:G:H3'     | 5:I:28:C:C6      | 2.36                     | 0.59              |
| 1:A:41:TYR:CD1   | 2:B:4:ILE:HG22   | 2.38                     | 0.58              |
| 2:B:80:PHE:CG    | 2:F:53:VAL:HG11  | 2.38                     | 0.58              |
| 2:C:99:VAL:O     | 2:C:103:GLN:HB2  | 2.03                     | 0.58              |
| 5:I:112:A:C4     | 5:I:123:A:C6     | 2.91                     | 0.58              |
| 1:A:256:ARG:NH1  | 5:I:78:C:H41     | 2.00                     | 0.58              |
| 5:I:109:A:N1     | 5:I:123:A:H5''   | 2.18                     | 0.58              |
| 5:I:103:A:N6     | 5:I:130:G:H1     | 2.01                     | 0.58              |
| 5:I:103:A:H61    | 5:I:130:G:H1     | 1.52                     | 0.58              |
| 2:B:105:LEU:O    | 2:B:109:VAL:HG23 | 2.04                     | 0.58              |
| 2:E:48:CYS:O     | 2:E:52:GLN:HB2   | 2.04                     | 0.58              |
| 1:A:127:ARG:HD2  | 1:A:267:PRO:HA   | 1.86                     | 0.58              |
| 2:D:36:ARG:O     | 2:D:37:LYS:C     | 2.46                     | 0.58              |
| 2:E:31:ALA:HB2   | 2:E:45:PHE:CE2   | 2.39                     | 0.58              |
| 1:A:58:TYR:CE2   | 1:A:86:VAL:HG11  | 2.39                     | 0.58              |
| 1:A:108:ALA:HA   | 1:A:213:TYR:CD1  | 2.38                     | 0.58              |
| 5:I:100:A:C2     | 5:I:130:G:C8     | 2.91                     | 0.58              |
| 5:I:109:A:H8     | 5:I:109:A:OP1    | 1.86                     | 0.58              |
| 2:C:50:LEU:HD13  | 2:D:81:TRP:CH2   | 2.39                     | 0.58              |
| 2:E:34:ILE:CD1   | 2:E:85:LEU:HG    | 2.34                     | 0.58              |
| 1:A:245:LYS:O    | 1:A:309:TRP:HZ3  | 1.87                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:36:ARG:O     | 2:C:37:LYS:C     | 2.47                     | 0.58              |
| 1:A:13:THR:OG1   | 1:A:54:LYS:HG3   | 2.04                     | 0.57              |
| 1:A:221:GLY:CA   | 1:A:227:LEU:HD11 | 2.33                     | 0.57              |
| 2:C:90:LYS:CB    | 2:C:91:PRO:HD2   | 2.33                     | 0.57              |
| 2:D:16:ILE:HG12  | 2:D:109:VAL:HG23 | 1.86                     | 0.57              |
| 2:E:34:ILE:HG23  | 2:E:93:ALA:HB1   | 1.84                     | 0.57              |
| 3:G:372:G:H5''   | 5:I:82:C:H5'     | 1.86                     | 0.57              |
| 1:A:18:LEU:HD13  | 1:A:50:GLN:HA    | 1.86                     | 0.57              |
| 1:A:108:ALA:HA   | 1:A:213:TYR:CE1  | 2.38                     | 0.57              |
| 2:B:13:GLN:CB    | 2:B:60:GLY:HA3   | 2.33                     | 0.57              |
| 2:F:85:LEU:HD23  | 2:F:88:ILE:HD12  | 1.86                     | 0.57              |
| 1:A:107:TYR:CZ   | 1:A:121:HIS:HB2  | 2.39                     | 0.57              |
| 2:D:24:ILE:HD11  | 2:D:53:VAL:HG21  | 1.85                     | 0.57              |
| 1:A:159:ILE:HG13 | 1:A:168:LEU:CD1  | 2.34                     | 0.57              |
| 2:D:26:TYR:CE2   | 2:D:30:ILE:HD11  | 2.40                     | 0.57              |
| 1:A:60:ARG:HH12  | 1:A:173:PRO:HD3  | 1.70                     | 0.57              |
| 1:A:139:PHE:HZ   | 1:A:197:VAL:HG11 | 1.69                     | 0.57              |
| 2:F:68:LEU:HD21  | 2:F:116:TRP:CD2  | 2.40                     | 0.57              |
| 1:A:126:LEU:HD11 | 1:A:258:ILE:HD12 | 1.85                     | 0.57              |
| 2:C:88:ILE:O     | 2:C:89:GLN:C     | 2.47                     | 0.57              |
| 1:A:49:LEU:HD13  | 2:B:1:MET:HE3    | 1.85                     | 0.57              |
| 1:A:274:LYS:NZ   | 1:A:278:LYS:NZ   | 2.52                     | 0.57              |
| 2:B:61:LYS:HZ3   | 2:C:76:ALA:HB2   | 1.68                     | 0.57              |
| 2:B:86:ALA:CB    | 2:B:99:VAL:HG21  | 2.35                     | 0.57              |
| 5:I:27:G:C8      | 5:I:27:G:H5''    | 2.39                     | 0.57              |
| 5:I:29:G:H5''    | 5:I:29:G:C8      | 2.39                     | 0.57              |
| 1:A:134:PHE:CD1  | 1:A:258:ILE:HG12 | 2.40                     | 0.56              |
| 1:A:284:VAL:HG21 | 1:A:319:MET:HE3  | 1.87                     | 0.56              |
| 1:A:115:THR:HA   | 1:A:261:LEU:HD13 | 1.87                     | 0.56              |
| 1:A:216:ASP:N    | 1:A:311:ASP:OD2  | 2.37                     | 0.56              |
| 1:A:231:PHE:HE1  | 1:A:246:ILE:HG21 | 1.69                     | 0.56              |
| 1:A:247:SER:HB3  | 1:A:309:TRP:CH2  | 2.40                     | 0.56              |
| 2:D:68:LEU:HD12  | 2:D:113:LEU:HD11 | 1.87                     | 0.56              |
| 2:E:34:ILE:HD11  | 2:E:45:PHE:CD2   | 2.40                     | 0.56              |
| 2:B:6:GLU:OE1    | 2:B:61:LYS:NZ    | 2.35                     | 0.56              |
| 2:B:47:LYS:NZ    | 2:C:43:GLU:OE2   | 2.35                     | 0.56              |
| 2:B:76:ALA:HB3   | 2:F:57:ILE:HG21  | 1.87                     | 0.56              |
| 2:C:28:TYR:CE1   | 2:D:41:ALA:HB2   | 2.40                     | 0.56              |
| 2:E:20:TYR:OH    | 2:E:49:LEU:HA    | 2.06                     | 0.56              |
| 2:F:52:GLN:HE22  | 2:F:71:ALA:HA    | 1.69                     | 0.56              |
| 5:I:110:U:H2'    | 5:I:122:G:O6     | 2.06                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:266:TRP:O    | 1:A:267:PRO:C    | 2.47                     | 0.56              |
| 2:B:88:ILE:CG2   | 2:F:25:SER:HA    | 2.34                     | 0.56              |
| 2:B:100:GLU:O    | 2:B:104:VAL:HG23 | 2.06                     | 0.56              |
| 2:D:21:GLU:OE2   | 2:E:80:PHE:CD1   | 2.58                     | 0.56              |
| 2:D:47:LYS:NZ    | 2:E:43:GLU:OE2   | 2.30                     | 0.56              |
| 2:D:50:LEU:HD21  | 2:E:84:PHE:CZ    | 2.41                     | 0.56              |
| 2:F:31:ALA:HA    | 2:F:34:ILE:HG13  | 1.87                     | 0.56              |
| 2:B:5:GLU:HA     | 2:B:9:LYS:NZ     | 2.20                     | 0.56              |
| 2:D:26:TYR:O     | 2:D:30:ILE:HG13  | 2.06                     | 0.56              |
| 1:A:126:LEU:HD23 | 1:A:131:ALA:HB3  | 1.87                     | 0.56              |
| 1:A:274:LYS:NZ   | 1:A:278:LYS:HZ3  | 2.03                     | 0.56              |
| 2:B:27:LEU:HA    | 2:B:30:ILE:HG12  | 1.87                     | 0.56              |
| 2:C:85:LEU:HD23  | 2:C:88:ILE:CD1   | 2.36                     | 0.56              |
| 1:A:53:LEU:HD23  | 1:A:58:TYR:HB2   | 1.88                     | 0.55              |
| 5:I:106:U:H2'    | 5:I:107:C:C6     | 2.41                     | 0.55              |
| 1:A:143:PHE:CZ   | 1:A:313:HIS:CG   | 2.94                     | 0.55              |
| 2:E:19:ARG:HG3   | 2:E:112:ILE:CD1  | 2.37                     | 0.55              |
| 5:I:26:G:H2'     | 5:I:27:G:C8      | 2.41                     | 0.55              |
| 2:B:88:ILE:HG21  | 2:F:24:ILE:HG22  | 1.87                     | 0.55              |
| 2:C:36:ARG:O     | 2:C:39:GLY:N     | 2.39                     | 0.55              |
| 2:D:13:GLN:NE2   | 2:D:119:ARG:HH12 | 2.04                     | 0.55              |
| 2:D:31:ALA:HB2   | 2:D:45:PHE:CE2   | 2.41                     | 0.55              |
| 2:D:32:GLN:NE2   | 5:I:7:U:H3       | 2.05                     | 0.55              |
| 2:D:85:LEU:HD12  | 2:D:94:MET:CE    | 2.37                     | 0.55              |
| 2:F:45:PHE:CD1   | 2:F:81:TRP:HB3   | 2.41                     | 0.55              |
| 2:F:73:ALA:O     | 2:F:77:MET:N     | 2.28                     | 0.55              |
| 2:C:52:GLN:OE1   | 2:C:75:LEU:N     | 2.39                     | 0.55              |
| 5:I:5:G:H5''     | 5:I:5:G:C8       | 2.40                     | 0.55              |
| 5:I:102:A:C6     | 5:I:103:A:C6     | 2.94                     | 0.55              |
| 1:A:4:ARG:O      | 1:A:160:HIS:ND1  | 2.39                     | 0.55              |
| 2:E:82:LEU:HD11  | 2:E:106:ILE:CD1  | 2.36                     | 0.55              |
| 2:B:61:LYS:HG3   | 2:C:73:ALA:CA    | 2.34                     | 0.55              |
| 2:E:59:ALA:C     | 2:E:116:TRP:CH2  | 2.82                     | 0.55              |
| 2:D:56:PHE:HE1   | 2:D:113:LEU:HD22 | 1.72                     | 0.55              |
| 1:A:29:LYS:HG3   | 1:A:84:ARG:HH12  | 1.72                     | 0.55              |
| 1:A:192:VAL:C    | 1:A:194:GLY:N    | 2.64                     | 0.55              |
| 2:B:4:ILE:HD13   | 2:C:107:ALA:CB   | 2.38                     | 0.55              |
| 1:A:142:PHE:O    | 1:A:146:ILE:HG13 | 2.07                     | 0.54              |
| 1:A:186:SER:O    | 1:A:189:PHE:N    | 2.40                     | 0.54              |
| 1:A:274:LYS:HD2  | 1:A:278:LYS:HZ2  | 1.69                     | 0.54              |
| 2:F:52:GLN:HA    | 2:F:55:LEU:HB2   | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:41:TYR:CE1   | 2:B:4:ILE:HG22   | 2.42                     | 0.54              |
| 1:A:277:VAL:HG13 | 1:A:315:LEU:HD11 | 1.89                     | 0.54              |
| 2:E:16:ILE:HD11  | 2:E:116:TRP:CE3  | 2.42                     | 0.54              |
| 5:I:1:C:O2'      | 5:I:2:A:H3'      | 2.07                     | 0.54              |
| 2:B:4:ILE:HD13   | 2:C:107:ALA:HB2  | 1.90                     | 0.54              |
| 1:A:215:ASP:H    | 1:A:311:ASP:CG   | 2.15                     | 0.54              |
| 1:A:12:ILE:CD1   | 1:A:164:THR:HG23 | 2.37                     | 0.54              |
| 1:A:143:PHE:HB3  | 1:A:179:ILE:HG22 | 1.89                     | 0.54              |
| 1:A:198:ASP:HB3  | 1:A:210:TRP:CH2  | 2.43                     | 0.54              |
| 1:A:247:SER:HB3  | 1:A:309:TRP:CZ3  | 2.43                     | 0.54              |
| 2:C:17:VAL:HG11  | 2:D:83:ARG:NH2   | 2.22                     | 0.54              |
| 5:I:101:A:H62    | 5:I:132:G:N2     | 2.03                     | 0.54              |
| 1:A:305:GLY:O    | 1:A:308:GLN:HG2  | 2.08                     | 0.54              |
| 2:D:27:LEU:HD23  | 2:D:30:ILE:HD12  | 1.90                     | 0.54              |
| 2:D:43:GLU:HG2   | 2:E:40:VAL:CG2   | 2.36                     | 0.54              |
| 2:D:57:ILE:CG2   | 2:E:76:ALA:HB3   | 2.37                     | 0.54              |
| 1:A:41:TYR:CG    | 2:B:4:ILE:HG21   | 2.42                     | 0.54              |
| 1:A:136:LYS:HE2  | 1:A:216:ASP:CB   | 2.37                     | 0.54              |
| 1:A:154:MET:SD   | 1:A:193:TYR:HA   | 2.47                     | 0.54              |
| 1:A:187:GLN:H    | 1:A:313:HIS:HE1  | 1.56                     | 0.54              |
| 3:G:372:G:H2'    | 3:G:373:C:C6     | 2.43                     | 0.54              |
| 5:I:105:G:C6     | 5:I:106:U:C4     | 2.96                     | 0.54              |
| 5:I:129:G:N2     | 5:I:131:G:N7     | 2.54                     | 0.54              |
| 1:A:167:LEU:O    | 1:A:171:VAL:HB   | 2.08                     | 0.54              |
| 2:D:69:TYR:OH    | 2:D:121:ASN:ND2  | 2.40                     | 0.54              |
| 2:E:60:GLY:N     | 2:E:116:TRP:HH2  | 2.06                     | 0.54              |
| 2:F:82:LEU:CD1   | 2:F:106:ILE:HD12 | 2.30                     | 0.54              |
| 2:E:12:ASP:O     | 2:E:16:ILE:HG13  | 2.08                     | 0.54              |
| 5:I:9:U:H2'      | 5:I:10:G:C8      | 2.43                     | 0.54              |
| 1:A:137:SER:HB2  | 1:A:246:ILE:HG21 | 1.90                     | 0.53              |
| 1:A:182:GLY:HA3  | 1:A:320:GLU:CD   | 2.33                     | 0.53              |
| 2:F:27:LEU:HB3   | 2:F:49:LEU:HD22  | 1.90                     | 0.53              |
| 2:C:105:LEU:O    | 2:C:109:VAL:HG23 | 2.08                     | 0.53              |
| 1:A:207:GLN:CD   | 1:A:230:VAL:HG21 | 2.33                     | 0.53              |
| 1:A:139:PHE:O    | 1:A:309:TRP:HA   | 2.08                     | 0.53              |
| 1:A:143:PHE:N    | 1:A:143:PHE:CD1  | 2.76                     | 0.53              |
| 1:A:200:LEU:HD22 | 1:A:237:PHE:CB   | 2.37                     | 0.53              |
| 2:D:31:ALA:O     | 2:D:42:ARG:HG3   | 2.08                     | 0.53              |
| 5:I:125:A:H2'    | 5:I:126:G:O4'    | 2.08                     | 0.53              |
| 1:A:18:LEU:HD11  | 1:A:53:LEU:CD1   | 2.28                     | 0.53              |
| 1:A:197:VAL:HG21 | 1:A:217:ILE:HD12 | 1.91                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:38:HIS:ND1   | 2:F:28:TYR:OH    | 2.40                     | 0.53              |
| 1:A:104:PRO:HB3  | 5:I:131:G:H5'    | 1.89                     | 0.53              |
| 5:I:30:G:H2'     | 5:I:31:G:C8      | 2.43                     | 0.53              |
| 1:A:148:ARG:HB3  | 1:A:175:GLU:O    | 2.09                     | 0.53              |
| 2:C:28:TYR:CZ    | 2:D:41:ALA:HB2   | 2.44                     | 0.53              |
| 2:E:19:ARG:HG3   | 2:E:112:ILE:HD11 | 1.91                     | 0.53              |
| 1:A:13:THR:HG22  | 1:A:53:LEU:HB2   | 1.89                     | 0.53              |
| 2:B:80:PHE:CZ    | 2:F:24:ILE:HD13  | 2.43                     | 0.53              |
| 2:C:90:LYS:HG2   | 5:I:2:A:OP1      | 2.09                     | 0.53              |
| 1:A:308:GLN:CG   | 1:A:309:TRP:N    | 2.71                     | 0.52              |
| 2:F:52:GLN:OE1   | 2:F:74:GLY:HA3   | 2.10                     | 0.52              |
| 1:A:126:LEU:HG   | 1:A:220:LEU:CD1  | 2.39                     | 0.52              |
| 1:A:282:ARG:HH22 | 3:G:371:G:P      | 2.32                     | 0.52              |
| 2:C:57:ILE:HG21  | 2:D:76:ALA:CB    | 2.39                     | 0.52              |
| 1:A:24:LYS:HB3   | 1:A:88:HIS:CE1   | 2.44                     | 0.52              |
| 2:C:75:LEU:HD12  | 2:C:113:LEU:CD2  | 2.40                     | 0.52              |
| 2:C:92:HIS:H     | 2:C:92:HIS:HD2   | 1.58                     | 0.52              |
| 2:E:85:LEU:CD1   | 2:E:88:ILE:HD12  | 2.40                     | 0.52              |
| 1:A:94:VAL:HG13  | 1:A:98:PHE:CE2   | 2.45                     | 0.52              |
| 1:A:135:LEU:HD13 | 1:A:231:PHE:HB2  | 1.90                     | 0.52              |
| 1:A:159:ILE:HG13 | 1:A:168:LEU:HD11 | 1.91                     | 0.52              |
| 2:E:27:LEU:HD21  | 2:E:102:ALA:CB   | 2.40                     | 0.52              |
| 1:A:25:THR:OG1   | 1:A:85:LEU:HA    | 2.09                     | 0.52              |
| 1:A:41:TYR:CE2   | 2:C:79:ARG:HD3   | 2.45                     | 0.52              |
| 1:A:105:TYR:CE2  | 1:A:202:HIS:CE1  | 2.98                     | 0.52              |
| 2:C:94:MET:HB3   | 2:C:99:VAL:HG22  | 1.90                     | 0.52              |
| 1:A:41:TYR:CD1   | 2:B:4:ILE:CG2    | 2.92                     | 0.52              |
| 1:A:103:LEU:HD22 | 1:A:202:HIS:CG   | 2.45                     | 0.52              |
| 1:A:218:VAL:HG11 | 1:A:258:ILE:HD13 | 1.92                     | 0.52              |
| 2:D:21:GLU:OE2   | 2:E:80:PHE:HD1   | 1.93                     | 0.52              |
| 2:E:17:VAL:HG21  | 2:E:57:ILE:HG13  | 1.91                     | 0.52              |
| 2:F:45:PHE:CG    | 2:F:85:LEU:HD11  | 2.44                     | 0.52              |
| 5:I:14:A:N6      | 5:I:24:U:H3      | 2.07                     | 0.52              |
| 1:A:108:ALA:O    | 1:A:110:ARG:HG2  | 2.10                     | 0.52              |
| 1:A:133:HIS:CG   | 1:A:224:PRO:HB3  | 2.45                     | 0.52              |
| 2:B:61:LYS:HB2   | 2:C:73:ALA:HB2   | 1.92                     | 0.52              |
| 2:E:64:GLN:C     | 2:E:66:SER:H     | 2.18                     | 0.52              |
| 5:I:14:A:H61     | 5:I:24:U:H3      | 1.57                     | 0.52              |
| 1:A:265:ILE:HA   | 1:A:270:LYS:HB3  | 1.92                     | 0.51              |
| 2:D:68:LEU:HD11  | 2:D:116:TRP:CD2  | 2.45                     | 0.51              |
| 1:A:87:GLN:HG2   | 1:A:171:VAL:HG22 | 1.91                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:212:ARG:HB2  | 1:A:217:ILE:CG2  | 2.37                     | 0.51              |
| 1:A:271:LEU:HD11 | 5:I:86:U:H2'     | 1.92                     | 0.51              |
| 2:C:24:ILE:HD13  | 2:D:80:PHE:CZ    | 2.45                     | 0.51              |
| 2:F:75:LEU:CD1   | 2:F:113:LEU:HD12 | 2.36                     | 0.51              |
| 1:A:141:LYS:HE3  | 1:A:144:PRO:HB2  | 1.91                     | 0.51              |
| 1:A:204:GLU:O    | 1:A:205:LEU:HB2  | 2.10                     | 0.51              |
| 1:A:215:ASP:N    | 1:A:215:ASP:OD1  | 2.42                     | 0.51              |
| 2:D:85:LEU:HD22  | 2:D:89:GLN:NE2   | 2.24                     | 0.51              |
| 5:I:24:U:C4      | 5:I:25:U:C4      | 2.98                     | 0.51              |
| 1:A:39:LYS:CA    | 1:A:42:ASP:HB3   | 2.38                     | 0.51              |
| 1:A:103:LEU:CD1  | 1:A:202:HIS:HB3  | 2.41                     | 0.51              |
| 2:F:20:TYR:CG    | 2:F:56:PHE:HE2   | 2.27                     | 0.51              |
| 1:A:13:THR:O     | 1:A:50:GLN:NE2   | 2.44                     | 0.51              |
| 2:E:82:LEU:CD1   | 2:E:106:ILE:HD12 | 2.41                     | 0.51              |
| 2:F:42:ARG:O     | 2:F:43:GLU:C     | 2.50                     | 0.51              |
| 1:A:190:ALA:HB3  | 1:A:214:MET:HE3  | 1.92                     | 0.51              |
| 2:C:38:HIS:HB3   | 2:C:88:ILE:HD13  | 1.91                     | 0.51              |
| 1:A:36:LEU:HD12  | 2:B:11:TYR:HE1   | 1.75                     | 0.51              |
| 1:A:275:SER:OG   | 5:I:81:A:N1      | 2.44                     | 0.51              |
| 2:F:98:GLN:O     | 2:F:102:ALA:N    | 2.44                     | 0.51              |
| 1:A:139:PHE:CZ   | 1:A:197:VAL:HG21 | 2.46                     | 0.51              |
| 1:A:139:PHE:HD1  | 1:A:246:ILE:HG12 | 1.76                     | 0.51              |
| 1:A:123:GLN:HB2  | 1:A:265:ILE:CG2  | 2.41                     | 0.51              |
| 2:D:53:VAL:HG11  | 2:E:80:PHE:CG    | 2.46                     | 0.51              |
| 2:D:53:VAL:HG11  | 2:E:80:PHE:CD1   | 2.46                     | 0.51              |
| 4:H:118:U:H2'    | 4:H:119:G:C8     | 2.45                     | 0.51              |
| 2:C:40:VAL:HA    | 2:C:43:GLU:HG2   | 1.93                     | 0.50              |
| 2:D:17:VAL:O     | 2:D:21:GLU:HG2   | 2.11                     | 0.50              |
| 1:A:223:ASP:O    | 1:A:226:GLU:N    | 2.44                     | 0.50              |
| 2:D:27:LEU:HD11  | 2:D:82:LEU:HD21  | 1.93                     | 0.50              |
| 1:A:185:THR:O    | 1:A:186:SER:C    | 2.54                     | 0.50              |
| 1:A:213:TYR:CD2  | 1:A:213:TYR:O    | 2.65                     | 0.50              |
| 1:A:218:VAL:CG1  | 1:A:258:ILE:HD13 | 2.42                     | 0.50              |
| 2:C:21:GLU:OE1   | 2:D:88:ILE:HD11  | 2.12                     | 0.50              |
| 2:C:34:ILE:HB    | 2:C:42:ARG:HB2   | 1.94                     | 0.50              |
| 5:I:28:C:H2'     | 5:I:29:G:C8      | 2.46                     | 0.50              |
| 2:C:16:ILE:HD12  | 2:C:109:VAL:HG13 | 1.92                     | 0.50              |
| 1:A:265:ILE:HG23 | 1:A:270:LYS:CB   | 2.40                     | 0.50              |
| 2:B:34:ILE:O     | 2:B:35:PRO:O     | 2.30                     | 0.50              |
| 2:D:28:TYR:CE1   | 2:D:32:GLN:HG3   | 2.47                     | 0.50              |
| 1:A:187:GLN:N    | 1:A:313:HIS:HE1  | 2.10                     | 0.50              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:201:LEU:HG  | 1:A:234:LEU:HD11 | 1.94                     | 0.50              |
| 2:B:38:HIS:ND1  | 2:F:28:TYR:CE2   | 2.78                     | 0.50              |
| 2:D:30:ILE:HD13 | 2:D:98:GLN:HB3   | 1.94                     | 0.50              |
| 2:E:38:HIS:CG   | 2:E:88:ILE:HD13  | 2.47                     | 0.50              |
| 5:I:26:G:C4     | 5:I:27:G:C8      | 3.00                     | 0.50              |
| 2:B:85:LEU:O    | 2:B:93:ALA:HB3   | 2.11                     | 0.50              |
| 2:E:26:TYR:CZ   | 2:E:30:ILE:HD11  | 2.47                     | 0.50              |
| 2:F:98:GLN:HA   | 2:F:101:THR:OG1  | 2.11                     | 0.50              |
| 2:F:100:GLU:O   | 2:F:104:VAL:HG23 | 2.12                     | 0.50              |
| 1:A:109:CYS:H   | 1:A:314:ASN:HD21 | 1.59                     | 0.50              |
| 2:C:72:ASP:N    | 2:C:113:LEU:HD21 | 2.26                     | 0.50              |
| 2:D:85:LEU:HB2  | 2:D:94:MET:HE3   | 1.94                     | 0.50              |
| 2:F:105:LEU:O   | 2:F:109:VAL:HG23 | 2.12                     | 0.50              |
| 1:A:33:TRP:HH2  | 2:B:9:LYS:HB3    | 1.76                     | 0.49              |
| 1:A:154:MET:C   | 1:A:156:ASP:H    | 2.20                     | 0.49              |
| 1:A:190:ALA:C   | 1:A:192:VAL:N    | 2.70                     | 0.49              |
| 1:A:215:ASP:N   | 1:A:311:ASP:OD2  | 2.45                     | 0.49              |
| 1:A:261:LEU:O   | 1:A:263:TYR:HD1  | 1.95                     | 0.49              |
| 2:C:35:PRO:HG2  | 2:C:91:PRO:HB2   | 1.93                     | 0.49              |
| 2:F:40:VAL:O    | 2:F:44:MET:HG3   | 2.12                     | 0.49              |
| 5:I:101:A:H2'   | 5:I:102:A:C8     | 2.47                     | 0.49              |
| 1:A:19:LEU:O    | 1:A:20:ASP:C     | 2.56                     | 0.49              |
| 2:D:28:TYR:CZ   | 2:D:32:GLN:NE2   | 2.81                     | 0.49              |
| 2:E:26:TYR:CE2  | 2:E:101:THR:HB   | 2.47                     | 0.49              |
| 5:I:96:C:H2'    | 5:I:97:G:C8      | 2.47                     | 0.49              |
| 2:C:75:LEU:HD12 | 2:C:113:LEU:HD23 | 1.95                     | 0.49              |
| 2:D:91:PRO:O    | 2:D:93:ALA:N     | 2.46                     | 0.49              |
| 2:F:68:LEU:HD21 | 2:F:116:TRP:CE2  | 2.47                     | 0.49              |
| 1:A:109:CYS:N   | 1:A:314:ASN:HD21 | 2.11                     | 0.49              |
| 2:C:87:GLY:O    | 2:C:89:GLN:N     | 2.45                     | 0.49              |
| 2:C:95:THR:OG1  | 2:C:98:GLN:HG3   | 2.12                     | 0.49              |
| 2:D:68:LEU:HD21 | 2:D:116:TRP:CE2  | 2.47                     | 0.49              |
| 2:F:34:ILE:HG22 | 2:F:38:HIS:HB2   | 1.95                     | 0.49              |
| 1:A:5:HIS:HB3   | 1:A:8:LEU:HD21   | 1.94                     | 0.49              |
| 1:A:109:CYS:H   | 1:A:314:ASN:ND2  | 2.10                     | 0.49              |
| 2:C:17:VAL:O    | 2:C:21:GLU:HG2   | 2.12                     | 0.49              |
| 2:D:36:ARG:O    | 2:D:39:GLY:N     | 2.45                     | 0.49              |
| 1:A:33:TRP:HH2  | 2:B:9:LYS:CB     | 2.25                     | 0.49              |
| 1:A:134:PHE:HB2 | 1:A:220:LEU:HD23 | 1.94                     | 0.49              |
| 2:D:40:VAL:O    | 2:D:44:MET:HG3   | 2.12                     | 0.49              |
| 1:A:50:GLN:O    | 1:A:54:LYS:HB2   | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:139:PHE:HB2  | 1:A:215:ASP:HB3  | 1.93                     | 0.49              |
| 1:A:190:ALA:C    | 1:A:192:VAL:H    | 2.19                     | 0.49              |
| 1:A:264:ARG:HB2  | 1:A:266:TRP:HZ3  | 1.78                     | 0.49              |
| 2:B:5:GLU:HA     | 2:B:9:LYS:HZ1    | 1.78                     | 0.49              |
| 2:D:90:LYS:O     | 2:D:92:HIS:N     | 2.45                     | 0.49              |
| 2:E:100:GLU:O    | 2:E:104:VAL:HG23 | 2.13                     | 0.49              |
| 1:A:45:ASN:OD1   | 2:B:3:PRO:HA     | 2.13                     | 0.49              |
| 1:A:58:TYR:CE1   | 1:A:86:VAL:HG21  | 2.47                     | 0.49              |
| 1:A:107:TYR:CZ   | 1:A:121:HIS:CB   | 2.95                     | 0.49              |
| 1:A:141:LYS:CB   | 1:A:308:GLN:HB2  | 2.43                     | 0.49              |
| 2:B:53:VAL:HG11  | 2:C:80:PHE:CG    | 2.47                     | 0.49              |
| 1:A:105:TYR:CE1  | 1:A:121:HIS:CE1  | 3.01                     | 0.49              |
| 1:A:146:ILE:HG12 | 1:A:193:TYR:CD2  | 2.36                     | 0.49              |
| 2:D:87:GLY:N     | 2:D:92:HIS:HB3   | 2.27                     | 0.49              |
| 5:I:35:G:C5      | 5:I:36:C:H2'     | 2.48                     | 0.49              |
| 1:A:30:ARG:HA    | 1:A:35:TYR:CD2   | 2.48                     | 0.48              |
| 2:B:59:ALA:HA    | 2:B:67:LYS:HB2   | 1.94                     | 0.48              |
| 2:C:34:ILE:HG12  | 2:C:93:ALA:HB2   | 1.94                     | 0.48              |
| 3:G:372:G:H5''   | 5:I:82:C:C5'     | 2.42                     | 0.48              |
| 1:A:273:ARG:C    | 1:A:274:LYS:HG3  | 2.37                     | 0.48              |
| 1:A:194:GLY:O    | 1:A:197:VAL:HG22 | 2.13                     | 0.48              |
| 1:A:305:GLY:HA2  | 1:A:308:GLN:CD   | 2.37                     | 0.48              |
| 2:B:57:ILE:HG21  | 2:C:76:ALA:HB3   | 1.95                     | 0.48              |
| 2:D:16:ILE:HD11  | 2:D:113:LEU:HB2  | 1.95                     | 0.48              |
| 1:A:33:TRP:CH2   | 2:B:9:LYS:HB3    | 2.47                     | 0.48              |
| 2:C:88:ILE:O     | 2:C:88:ILE:HG22  | 2.14                     | 0.48              |
| 1:A:105:TYR:CD1  | 1:A:121:HIS:NE2  | 2.82                     | 0.48              |
| 1:A:213:TYR:O    | 1:A:214:MET:CB   | 2.61                     | 0.48              |
| 1:A:217:ILE:O    | 1:A:218:VAL:C    | 2.52                     | 0.48              |
| 2:B:80:PHE:CZ    | 2:B:84:PHE:HB2   | 2.48                     | 0.48              |
| 2:D:52:GLN:OE1   | 2:D:75:LEU:HG    | 2.14                     | 0.48              |
| 5:I:76:G:C5      | 5:I:77:G:H1'     | 2.48                     | 0.48              |
| 1:A:271:LEU:HD21 | 5:I:87:U:H5'     | 1.96                     | 0.48              |
| 2:C:90:LYS:HD2   | 2:C:90:LYS:H     | 1.78                     | 0.48              |
| 1:A:53:LEU:HD21  | 1:A:86:VAL:CG2   | 2.44                     | 0.48              |
| 1:A:189:PHE:O    | 1:A:192:VAL:HB   | 2.14                     | 0.48              |
| 2:B:72:ASP:N     | 2:B:113:LEU:HD21 | 2.29                     | 0.48              |
| 2:E:50:LEU:O     | 2:F:44:MET:HE1   | 2.14                     | 0.48              |
| 2:F:13:GLN:HE21  | 2:F:116:TRP:HB2  | 1.78                     | 0.48              |
| 2:F:27:LEU:HD12  | 2:F:30:ILE:HD11  | 1.95                     | 0.48              |
| 1:A:94:VAL:O     | 1:A:97:ILE:HG12  | 2.13                     | 0.48              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:B:60:GLY:HA2  | 2:B:116:TRP:HZ2  | 1.78                     | 0.48              |
| 1:A:143:PHE:HZ  | 1:A:214:MET:CE   | 2.24                     | 0.48              |
| 1:A:166:ARG:O   | 1:A:170:VAL:HG23 | 2.14                     | 0.48              |
| 2:B:27:LEU:O    | 2:B:31:ALA:N     | 2.47                     | 0.48              |
| 2:D:34:ILE:HG21 | 2:D:89:GLN:NE2   | 2.28                     | 0.48              |
| 2:E:89:GLN:HB3  | 2:E:91:PRO:HD2   | 1.96                     | 0.48              |
| 1:A:274:LYS:HZ2 | 1:A:278:LYS:HZ3  | 1.60                     | 0.48              |
| 2:C:81:TRP:O    | 2:C:85:LEU:HD12  | 2.13                     | 0.48              |
| 2:C:85:LEU:HD23 | 2:C:88:ILE:HD11  | 1.96                     | 0.48              |
| 2:D:91:PRO:O    | 2:D:92:HIS:C     | 2.56                     | 0.48              |
| 2:F:30:ILE:HG21 | 2:F:98:GLN:NE2   | 2.28                     | 0.48              |
| 5:I:10:G:C6     | 5:I:11:C:C4      | 3.02                     | 0.48              |
| 1:A:108:ALA:O   | 1:A:109:CYS:C    | 2.56                     | 0.47              |
| 1:A:271:LEU:CD1 | 5:I:86:U:H2'     | 2.44                     | 0.47              |
| 2:F:27:LEU:HB3  | 2:F:49:LEU:CD2   | 2.43                     | 0.47              |
| 2:F:30:ILE:HA   | 2:F:33:SER:HB3   | 1.96                     | 0.47              |
| 5:I:104:C:O2    | 5:I:130:G:N2     | 2.47                     | 0.47              |
| 1:A:296:LEU:O   | 1:A:300:LEU:HB2  | 2.14                     | 0.47              |
| 2:D:19:ARG:HG3  | 2:D:112:ILE:HD11 | 1.95                     | 0.47              |
| 2:F:52:GLN:HE22 | 2:F:71:ALA:CA    | 2.26                     | 0.47              |
| 2:B:38:HIS:ND1  | 2:F:28:TYR:HE2   | 2.12                     | 0.47              |
| 2:D:28:TYR:CD2  | 2:E:84:PHE:HZ    | 2.32                     | 0.47              |
| 5:I:5:G:C2'     | 5:I:6:C:H5'      | 2.43                     | 0.47              |
| 1:A:31:ARG:O    | 2:B:11:TYR:OH    | 2.31                     | 0.47              |
| 1:A:187:GLN:HG3 | 1:A:313:HIS:CE1  | 2.50                     | 0.47              |
| 2:B:82:LEU:HD11 | 2:B:106:ILE:CD1  | 2.44                     | 0.47              |
| 2:D:113:LEU:O   | 2:D:117:ILE:HG12 | 2.14                     | 0.47              |
| 2:F:34:ILE:HB   | 2:F:42:ARG:HB2   | 1.95                     | 0.47              |
| 2:F:35:PRO:HG3  | 2:F:92:HIS:CD2   | 2.49                     | 0.47              |
| 2:C:89:GLN:HG2  | 5:I:42:C:O4'     | 2.13                     | 0.47              |
| 2:D:68:LEU:HD12 | 2:D:113:LEU:CD1  | 2.45                     | 0.47              |
| 2:E:20:TYR:OH   | 2:E:49:LEU:HD12  | 2.13                     | 0.47              |
| 5:I:98:G:C2     | 5:I:134:C:C2     | 3.02                     | 0.47              |
| 1:A:63:TYR:CE1  | 1:A:79:LEU:HG    | 2.49                     | 0.47              |
| 1:A:108:ALA:HB2 | 1:A:213:TYR:CA   | 2.44                     | 0.47              |
| 1:A:123:GLN:HB2 | 1:A:265:ILE:HG21 | 1.96                     | 0.47              |
| 2:B:24:ILE:HD11 | 2:B:53:VAL:CG2   | 2.45                     | 0.47              |
| 2:B:44:MET:HE2  | 2:B:44:MET:HB3   | 1.77                     | 0.47              |
| 2:D:87:GLY:HA2  | 2:D:92:HIS:ND1   | 2.29                     | 0.47              |
| 2:E:34:ILE:HG23 | 2:E:93:ALA:CB    | 2.44                     | 0.47              |
| 1:A:107:TYR:N   | 1:A:212:ARG:O    | 2.42                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:152:TYR:CE2  | 1:A:172:LEU:HD23 | 2.50                     | 0.47              |
| 1:A:216:ASP:CG   | 1:A:311:ASP:CG   | 2.83                     | 0.47              |
| 1:A:228:ARG:HA   | 1:A:251:VAL:HG21 | 1.97                     | 0.47              |
| 1:A:304:SER:HA   | 1:A:316:PHE:HZ   | 1.80                     | 0.47              |
| 1:A:311:ASP:OD1  | 1:A:311:ASP:N    | 2.46                     | 0.47              |
| 2:B:13:GLN:HB3   | 2:B:60:GLY:HA3   | 1.95                     | 0.47              |
| 2:B:18:GLU:O     | 2:B:21:GLU:HB2   | 2.15                     | 0.47              |
| 2:D:87:GLY:O     | 2:D:92:HIS:ND1   | 2.46                     | 0.47              |
| 2:E:99:VAL:O     | 2:E:103:GLN:HG2  | 2.15                     | 0.47              |
| 2:F:41:ALA:HB1   | 2:F:84:PHE:HE2   | 1.79                     | 0.47              |
| 5:I:10:G:C6      | 5:I:29:G:C6      | 3.03                     | 0.47              |
| 5:I:104:C:H2'    | 5:I:105:G:O4'    | 2.15                     | 0.47              |
| 2:C:92:HIS:CD2   | 2:C:92:HIS:N     | 2.80                     | 0.47              |
| 2:E:37:LYS:HE3   | 5:I:7:U:O2       | 2.15                     | 0.47              |
| 1:A:126:LEU:HD21 | 1:A:220:LEU:HD22 | 1.97                     | 0.47              |
| 1:A:155:ILE:CG2  | 1:A:168:LEU:HD13 | 2.45                     | 0.47              |
| 1:A:187:GLN:N    | 1:A:313:HIS:CE1  | 2.82                     | 0.47              |
| 1:A:274:LYS:O    | 1:A:275:SER:HB3  | 2.14                     | 0.47              |
| 2:B:26:TYR:OH    | 2:B:98:GLN:HG2   | 2.15                     | 0.47              |
| 2:E:27:LEU:CD1   | 2:E:82:LEU:HD21  | 2.45                     | 0.47              |
| 1:A:13:THR:HG22  | 1:A:53:LEU:CB    | 2.45                     | 0.47              |
| 1:A:143:PHE:HD2  | 1:A:179:ILE:CG2  | 2.27                     | 0.47              |
| 1:A:151:LEU:HD21 | 1:A:189:PHE:CD2  | 2.50                     | 0.47              |
| 2:D:95:THR:O     | 2:D:99:VAL:HG23  | 2.15                     | 0.47              |
| 5:I:11:C:H2'     | 5:I:12:C:O4'     | 2.14                     | 0.47              |
| 1:A:109:CYS:HB3  | 1:A:314:ASN:OD1  | 2.15                     | 0.46              |
| 1:A:313:HIS:O    | 1:A:314:ASN:C    | 2.58                     | 0.46              |
| 5:I:79:G:H2'     | 5:I:80:A:C8      | 2.50                     | 0.46              |
| 1:A:197:VAL:CG2  | 1:A:217:ILE:HD12 | 2.46                     | 0.46              |
| 1:A:221:GLY:HA3  | 1:A:227:LEU:CD2  | 2.39                     | 0.46              |
| 2:D:46:LEU:HB2   | 2:E:40:VAL:HG11  | 1.97                     | 0.46              |
| 5:I:15:C:N4      | 5:I:24:U:O2'     | 2.47                     | 0.46              |
| 1:A:103:LEU:HD13 | 1:A:202:HIS:CB   | 2.43                     | 0.46              |
| 1:A:119:VAL:HG11 | 1:A:263:TYR:CD1  | 2.50                     | 0.46              |
| 1:A:212:ARG:HA   | 1:A:216:ASP:O    | 2.15                     | 0.46              |
| 2:D:82:LEU:HB3   | 2:D:99:VAL:HG13  | 1.98                     | 0.46              |
| 2:E:23:VAL:HG12  | 2:E:27:LEU:HD12  | 1.96                     | 0.46              |
| 5:I:69:C:H2'     | 5:I:70:U:C6      | 2.50                     | 0.46              |
| 5:I:109:A:O3'    | 5:I:110:U:H4'    | 2.15                     | 0.46              |
| 2:C:85:LEU:HB3   | 2:C:93:ALA:CB    | 2.43                     | 0.46              |
| 1:A:4:ARG:NH2    | 5:I:111:U:O4     | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:141:LYS:HA   | 1:A:308:GLN:CB   | 2.27                     | 0.46              |
| 2:B:106:ILE:O    | 2:B:110:GLY:N    | 2.46                     | 0.46              |
| 2:C:31:ALA:O     | 2:C:42:ARG:HG3   | 2.14                     | 0.46              |
| 2:D:99:VAL:HG12  | 2:D:103:GLN:OE1  | 2.16                     | 0.46              |
| 5:I:105:G:H1'    | 5:I:129:G:N2     | 2.31                     | 0.46              |
| 1:A:19:LEU:HD21  | 1:A:43:LEU:HD22  | 1.98                     | 0.46              |
| 1:A:25:THR:HG22  | 1:A:81:PHE:CE1   | 2.50                     | 0.46              |
| 1:A:42:ASP:HA    | 1:A:45:ASN:HB2   | 1.98                     | 0.46              |
| 1:A:200:LEU:HD13 | 1:A:237:PHE:CG   | 2.49                     | 0.46              |
| 2:B:44:MET:CE    | 2:F:47:LYS:HA    | 2.45                     | 0.46              |
| 5:I:25:U:C2      | 5:I:26:G:C8      | 3.03                     | 0.46              |
| 1:A:8:LEU:HD12   | 1:A:159:ILE:HG23 | 1.97                     | 0.46              |
| 1:A:109:CYS:CA   | 1:A:314:ASN:HD21 | 2.29                     | 0.46              |
| 1:A:139:PHE:CZ   | 1:A:217:ILE:HD11 | 2.50                     | 0.46              |
| 2:B:50:LEU:HD21  | 2:C:84:PHE:CE1   | 2.51                     | 0.46              |
| 5:I:26:G:H2'     | 5:I:27:G:H8      | 1.81                     | 0.46              |
| 1:A:187:GLN:CA   | 1:A:313:HIS:CE1  | 2.98                     | 0.46              |
| 2:B:7:ALA:O      | 2:B:8:THR:C      | 2.59                     | 0.46              |
| 2:C:34:ILE:CG2   | 2:C:38:HIS:HB2   | 2.46                     | 0.46              |
| 2:E:53:VAL:HG12  | 2:E:57:ILE:HD12  | 1.98                     | 0.46              |
| 5:I:77:G:H5''    | 5:I:77:G:C8      | 2.50                     | 0.46              |
| 1:A:8:LEU:CD1    | 1:A:159:ILE:HD12 | 2.45                     | 0.46              |
| 1:A:192:VAL:O    | 1:A:195:GLY:N    | 2.49                     | 0.46              |
| 2:B:84:PHE:HA    | 2:B:88:ILE:HD12  | 1.98                     | 0.46              |
| 2:C:50:LEU:HD13  | 2:D:81:TRP:HH2   | 1.81                     | 0.46              |
| 2:C:89:GLN:CG    | 2:C:90:LYS:HE2   | 2.46                     | 0.46              |
| 1:A:198:ASP:CG   | 1:A:212:ARG:HE   | 2.24                     | 0.46              |
| 1:A:271:LEU:HD13 | 1:A:272:LEU:H    | 1.80                     | 0.46              |
| 1:A:273:ARG:HD2  | 1:A:273:ARG:HA   | 1.78                     | 0.46              |
| 2:C:43:GLU:HG3   | 2:C:44:MET:N     | 2.30                     | 0.46              |
| 1:A:41:TYR:CZ    | 2:C:79:ARG:NH1   | 2.84                     | 0.45              |
| 1:A:146:ILE:C    | 1:A:148:ARG:N    | 2.73                     | 0.45              |
| 2:C:16:ILE:HG21  | 2:C:116:TRP:HZ3  | 1.80                     | 0.45              |
| 2:C:90:LYS:HB3   | 2:C:91:PRO:HD2   | 1.96                     | 0.45              |
| 2:D:54:GLU:HB2   | 2:E:77:MET:HE2   | 1.98                     | 0.45              |
| 2:E:77:MET:O     | 2:E:81:TRP:CD1   | 2.69                     | 0.45              |
| 2:F:34:ILE:O     | 2:F:42:ARG:NH1   | 2.49                     | 0.45              |
| 2:B:16:ILE:HG12  | 2:B:109:VAL:HG13 | 1.98                     | 0.45              |
| 2:B:56:PHE:CD1   | 2:B:71:ALA:HB1   | 2.51                     | 0.45              |
| 2:E:37:LYS:HA    | 5:I:7:U:O4'      | 2.16                     | 0.45              |
| 5:I:107:C:H2'    | 5:I:108:G:O4'    | 2.15                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:57:ILE:O     | 2:B:61:LYS:HG2   | 2.16                     | 0.45              |
| 2:D:28:TYR:OH    | 2:D:32:GLN:NE2   | 2.50                     | 0.45              |
| 2:D:50:LEU:HD21  | 2:E:84:PHE:CE1   | 2.51                     | 0.45              |
| 5:I:73:U:H2'     | 5:I:75:C:C4      | 2.51                     | 0.45              |
| 1:A:38:PHE:HZ    | 1:A:46:LEU:HD23  | 1.81                     | 0.45              |
| 1:A:219:VAL:HG12 | 1:A:219:VAL:O    | 2.16                     | 0.45              |
| 2:E:31:ALA:O     | 2:E:42:ARG:HG3   | 2.16                     | 0.45              |
| 4:H:128:C:N3     | 5:I:46:A:H2      | 2.15                     | 0.45              |
| 5:I:100:A:H4'    | 5:I:101:A:C8     | 2.47                     | 0.45              |
| 1:A:132:THR:C    | 1:A:254:VAL:HG23 | 2.41                     | 0.45              |
| 1:A:140:SER:CA   | 1:A:309:TRP:CZ3  | 2.97                     | 0.45              |
| 1:A:274:LYS:O    | 1:A:276:SER:N    | 2.40                     | 0.45              |
| 2:B:60:GLY:HA2   | 2:B:116:TRP:CZ2  | 2.50                     | 0.45              |
| 2:B:37:LYS:HB2   | 2:B:37:LYS:HE2   | 1.78                     | 0.45              |
| 2:B:49:LEU:HA    | 2:B:78:LEU:HD13  | 1.99                     | 0.45              |
| 2:C:106:ILE:O    | 2:C:110:GLY:N    | 2.44                     | 0.45              |
| 1:A:4:ARG:O      | 1:A:160:HIS:CB   | 2.62                     | 0.45              |
| 1:A:105:TYR:CD1  | 1:A:121:HIS:CE1  | 3.05                     | 0.45              |
| 2:D:56:PHE:CD1   | 2:D:71:ALA:HB1   | 2.51                     | 0.45              |
| 2:F:20:TYR:HA    | 2:F:109:VAL:HG21 | 1.99                     | 0.45              |
| 1:A:39:LYS:O     | 1:A:40:GLU:C     | 2.60                     | 0.45              |
| 1:A:41:TYR:OH    | 2:C:79:ARG:NH1   | 2.50                     | 0.45              |
| 1:A:60:ARG:H     | 1:A:170:VAL:CG1  | 2.30                     | 0.45              |
| 1:A:208:ARG:HE   | 5:I:129:G:H5'    | 1.82                     | 0.45              |
| 2:B:9:LYS:HE2    | 2:B:14:MET:HE1   | 1.98                     | 0.45              |
| 2:D:28:TYR:CE2   | 2:D:50:LEU:HD11  | 2.52                     | 0.45              |
| 2:D:37:LYS:HE3   | 2:D:37:LYS:HB3   | 1.54                     | 0.45              |
| 1:A:103:LEU:CD2  | 1:A:104:PRO:HD2  | 2.43                     | 0.45              |
| 1:A:141:LYS:O    | 1:A:144:PRO:HD2  | 2.16                     | 0.45              |
| 2:B:75:LEU:HD21  | 2:B:109:VAL:HG12 | 1.99                     | 0.45              |
| 5:I:125:A:C2     | 5:I:126:G:H1'    | 2.52                     | 0.45              |
| 2:B:38:HIS:NE2   | 2:B:91:PRO:HD3   | 2.32                     | 0.45              |
| 2:D:28:TYR:CZ    | 2:E:88:ILE:HD11  | 2.52                     | 0.45              |
| 2:D:98:GLN:HA    | 2:D:101:THR:HG23 | 1.98                     | 0.45              |
| 2:E:15:LEU:HG    | 2:E:112:ILE:HD13 | 1.99                     | 0.45              |
| 2:E:26:TYR:CE2   | 2:E:30:ILE:HD11  | 2.52                     | 0.44              |
| 2:E:60:GLY:C     | 2:E:62:SER:H     | 2.25                     | 0.44              |
| 5:I:71:G:N2      | 5:I:79:G:H1'     | 2.33                     | 0.44              |
| 1:A:152:TYR:OH   | 1:A:172:LEU:HB3  | 2.18                     | 0.44              |
| 1:A:188:LEU:O    | 1:A:192:VAL:HG23 | 2.18                     | 0.44              |
| 1:A:269:HIS:HB3  | 5:I:90:A:H61     | 1.82                     | 0.44              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:B:52:GLN:OE1  | 2:B:74:GLY:HA3   | 2.17                     | 0.44              |
| 2:B:84:PHE:CE1  | 2:F:50:LEU:HD21  | 2.52                     | 0.44              |
| 2:B:90:LYS:HD3  | 2:B:90:LYS:HA    | 1.48                     | 0.44              |
| 2:F:108:GLU:O   | 2:F:112:ILE:HG13 | 2.18                     | 0.44              |
| 1:A:139:PHE:CD1 | 1:A:246:ILE:HG12 | 2.52                     | 0.44              |
| 2:B:12:ASP:HB3  | 2:B:116:TRP:CG   | 2.52                     | 0.44              |
| 2:C:35:PRO:HD2  | 2:C:38:HIS:HD2   | 1.82                     | 0.44              |
| 2:F:94:MET:HG3  | 2:F:98:GLN:HB2   | 1.99                     | 0.44              |
| 2:B:52:GLN:OE1  | 2:B:74:GLY:C     | 2.61                     | 0.44              |
| 2:E:28:TYR:HB3  | 2:E:29:PRO:HD3   | 2.00                     | 0.44              |
| 2:F:83:ARG:O    | 2:F:86:ALA:HB3   | 2.18                     | 0.44              |
| 1:A:90:LEU:C    | 1:A:92:ASN:H     | 2.26                     | 0.44              |
| 2:C:82:LEU:CD2  | 2:C:94:MET:SD    | 3.03                     | 0.44              |
| 2:C:91:PRO:O    | 2:C:93:ALA:N     | 2.50                     | 0.44              |
| 2:E:80:PHE:CE1  | 2:E:84:PHE:HB2   | 2.52                     | 0.44              |
| 2:F:27:LEU:HG   | 2:F:45:PHE:CZ    | 2.41                     | 0.44              |
| 2:F:31:ALA:HB2  | 2:F:45:PHE:CE2   | 2.52                     | 0.44              |
| 5:I:105:G:H2'   | 5:I:106:U:O4'    | 2.17                     | 0.44              |
| 2:B:80:PHE:CE1  | 2:B:84:PHE:HB2   | 2.52                     | 0.44              |
| 2:C:31:ALA:HB2  | 2:C:45:PHE:CE2   | 2.53                     | 0.44              |
| 1:A:3:LYS:O     | 1:A:4:ARG:HB2    | 2.18                     | 0.44              |
| 1:A:7:ASN:N     | 1:A:161:CYS:HB2  | 2.32                     | 0.44              |
| 1:A:241:ARG:HB3 | 1:A:242:LEU:HD23 | 1.98                     | 0.44              |
| 1:A:260:PHE:HB3 | 1:A:265:ILE:HD11 | 1.99                     | 0.44              |
| 2:C:34:ILE:CD1  | 2:C:85:LEU:HD22  | 2.46                     | 0.44              |
| 1:A:41:TYR:CG   | 2:B:4:ILE:CG2    | 3.01                     | 0.44              |
| 2:B:72:ASP:CA   | 2:B:113:LEU:HD21 | 2.48                     | 0.44              |
| 2:B:82:LEU:CD1  | 2:B:106:ILE:HD12 | 2.47                     | 0.44              |
| 5:I:29:G:H3'    | 5:I:30:G:H8      | 1.83                     | 0.44              |
| 5:I:76:G:C2     | 5:I:77:G:C8      | 3.06                     | 0.44              |
| 1:A:4:ARG:NH2   | 5:I:110:U:O2'    | 2.47                     | 0.44              |
| 1:A:5:HIS:O     | 1:A:159:ILE:O    | 2.36                     | 0.44              |
| 1:A:107:TYR:HE2 | 1:A:121:HIS:CD2  | 2.36                     | 0.44              |
| 2:B:56:PHE:O    | 2:B:59:ALA:HB3   | 2.17                     | 0.44              |
| 2:D:75:LEU:HD23 | 2:D:75:LEU:HA    | 1.86                     | 0.44              |
| 2:D:75:LEU:HD11 | 2:D:109:VAL:HG13 | 1.99                     | 0.44              |
| 2:E:36:ARG:O    | 2:E:37:LYS:C     | 2.60                     | 0.44              |
| 5:I:23:C:H2'    | 5:I:24:U:O4'     | 2.17                     | 0.44              |
| 5:I:112:A:C2    | 5:I:123:A:C2     | 3.06                     | 0.44              |
| 1:A:41:TYR:CZ   | 2:C:79:ARG:HD3   | 2.53                     | 0.43              |
| 1:A:46:LEU:HD21 | 1:A:85:LEU:HD11  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:98:PHE:CE1   | 1:A:158:LYS:HB3  | 2.52                     | 0.43              |
| 2:B:94:MET:HB3   | 2:B:94:MET:HE2   | 1.76                     | 0.43              |
| 2:C:23:VAL:HG11  | 2:C:78:LEU:HD21  | 1.99                     | 0.43              |
| 2:C:24:ILE:HD11  | 2:C:53:VAL:HG22  | 1.99                     | 0.43              |
| 2:E:20:TYR:HA    | 2:E:109:VAL:HG11 | 2.00                     | 0.43              |
| 5:I:27:G:C5      | 5:I:28:C:C4      | 3.06                     | 0.43              |
| 5:I:77:G:H5'     | 5:I:77:G:H8      | 1.81                     | 0.43              |
| 1:A:41:TYR:CD2   | 2:C:107:ALA:HB2  | 2.53                     | 0.43              |
| 1:A:60:ARG:HB2   | 1:A:170:VAL:HG12 | 2.00                     | 0.43              |
| 1:A:221:GLY:HA3  | 1:A:227:LEU:CD1  | 2.44                     | 0.43              |
| 1:A:266:TRP:CD1  | 1:A:268:THR:HB   | 2.54                     | 0.43              |
| 2:E:40:VAL:O     | 2:E:44:MET:HG3   | 2.18                     | 0.43              |
| 1:A:126:LEU:CD2  | 1:A:254:VAL:HG11 | 2.43                     | 0.43              |
| 2:F:27:LEU:HD12  | 2:F:27:LEU:HA    | 1.75                     | 0.43              |
| 1:A:17:ASN:HD21  | 1:A:92:ASN:HB2   | 1.82                     | 0.43              |
| 1:A:200:LEU:HG   | 1:A:200:LEU:O    | 2.18                     | 0.43              |
| 2:B:24:ILE:HD13  | 2:C:80:PHE:CZ    | 2.53                     | 0.43              |
| 2:E:27:LEU:HD21  | 2:E:102:ALA:HB2  | 1.98                     | 0.43              |
| 2:E:27:LEU:HD23  | 2:E:27:LEU:HA    | 1.74                     | 0.43              |
| 1:A:9:ILE:N      | 1:A:164:THR:OG1  | 2.51                     | 0.43              |
| 2:D:38:HIS:NE2   | 2:D:91:PRO:CD    | 2.79                     | 0.43              |
| 1:A:36:LEU:HD13  | 2:B:15:LEU:N     | 2.32                     | 0.43              |
| 1:A:123:GLN:O    | 1:A:126:LEU:HB2  | 2.19                     | 0.43              |
| 2:B:31:ALA:HB2   | 2:B:45:PHE:CE2   | 2.54                     | 0.43              |
| 2:B:54:GLU:O     | 2:B:58:VAL:HG22  | 2.19                     | 0.43              |
| 2:C:37:LYS:O     | 5:I:3:U:C4       | 2.72                     | 0.43              |
| 2:D:100:GLU:O    | 2:D:104:VAL:HG23 | 2.19                     | 0.43              |
| 2:E:46:LEU:HD23  | 2:E:46:LEU:HA    | 1.79                     | 0.43              |
| 5:I:9:U:H2'      | 5:I:10:G:H8      | 1.81                     | 0.43              |
| 1:A:126:LEU:HD13 | 1:A:267:PRO:HD3  | 2.01                     | 0.43              |
| 1:A:137:SER:HB2  | 1:A:246:ILE:CG2  | 2.48                     | 0.43              |
| 1:A:262:GLY:O    | 1:A:273:ARG:N    | 2.51                     | 0.43              |
| 1:A:305:GLY:O    | 1:A:308:GLN:CD   | 2.62                     | 0.43              |
| 2:C:34:ILE:HG12  | 2:C:93:ALA:CB    | 2.49                     | 0.43              |
| 2:D:44:MET:HE2   | 2:D:44:MET:HB3   | 1.62                     | 0.43              |
| 5:I:85:G:H1'     | 5:I:89:C:N4      | 2.33                     | 0.43              |
| 1:A:122:VAL:HB   | 1:A:265:ILE:HD13 | 2.01                     | 0.43              |
| 2:B:27:LEU:CD1   | 2:B:82:LEU:HD21  | 2.47                     | 0.43              |
| 2:C:30:ILE:HD12  | 2:C:98:GLN:OE1   | 2.18                     | 0.43              |
| 2:D:74:GLY:O     | 2:D:78:LEU:N     | 2.45                     | 0.43              |
| 2:D:85:LEU:CD2   | 2:D:89:GLN:NE2   | 2.82                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:128:C:H2'    | 4:H:129:U:O4'    | 2.19                     | 0.43              |
| 1:A:169:ARG:HG2  | 1:A:174:ASP:HB2  | 2.01                     | 0.43              |
| 2:E:19:ARG:HH21  | 2:E:108:GLU:HG3  | 1.82                     | 0.43              |
| 1:A:278:LYS:HB2  | 1:A:278:LYS:HE2  | 1.56                     | 0.43              |
| 2:B:20:TYR:OH    | 2:B:49:LEU:HD12  | 2.18                     | 0.43              |
| 2:B:20:TYR:CE2   | 2:B:52:GLN:HB3   | 2.54                     | 0.43              |
| 2:F:23:VAL:HG11  | 2:F:106:ILE:HG12 | 2.01                     | 0.43              |
| 5:I:29:G:C6      | 5:I:30:G:C5      | 3.07                     | 0.43              |
| 1:A:256:ARG:HH22 | 5:I:78:C:N4      | 2.17                     | 0.42              |
| 2:E:37:LYS:HD2   | 5:I:7:U:O4'      | 2.19                     | 0.42              |
| 2:E:87:GLY:N     | 5:I:19:A:H61     | 2.17                     | 0.42              |
| 5:I:15:C:H2'     | 5:I:16:G:O4'     | 2.19                     | 0.42              |
| 1:A:133:HIS:CD2  | 1:A:224:PRO:HB3  | 2.53                     | 0.42              |
| 1:A:259:ASN:ND2  | 1:A:264:ARG:HG2  | 2.33                     | 0.42              |
| 2:B:7:ALA:CB     | 2:C:117:ILE:HD13 | 2.49                     | 0.42              |
| 2:F:102:ALA:O    | 2:F:106:ILE:HG13 | 2.19                     | 0.42              |
| 5:I:26:G:C2      | 5:I:27:G:C4      | 3.07                     | 0.42              |
| 1:A:179:ILE:HD11 | 1:A:189:PHE:HB3  | 2.02                     | 0.42              |
| 1:A:192:VAL:O    | 1:A:194:GLY:N    | 2.53                     | 0.42              |
| 1:A:200:LEU:HD22 | 1:A:237:PHE:HB3  | 2.02                     | 0.42              |
| 2:E:65:VAL:HA    | 2:E:68:LEU:HD13  | 2.02                     | 0.42              |
| 5:I:112:A:H1'    | 5:I:123:A:N6     | 2.35                     | 0.42              |
| 1:A:275:SER:CB   | 5:I:81:A:N1      | 2.83                     | 0.42              |
| 2:B:57:ILE:CG2   | 2:C:76:ALA:HB3   | 2.49                     | 0.42              |
| 2:C:57:ILE:HD12  | 2:D:76:ALA:HB1   | 2.00                     | 0.42              |
| 2:D:13:GLN:N     | 2:D:60:GLY:HA3   | 2.34                     | 0.42              |
| 2:D:90:LYS:HD3   | 2:D:90:LYS:HA    | 1.85                     | 0.42              |
| 2:E:85:LEU:HD12  | 2:E:88:ILE:HD12  | 2.00                     | 0.42              |
| 5:I:115:G:N2     | 5:I:117:A:H3'    | 2.34                     | 0.42              |
| 1:A:223:ASP:C    | 1:A:225:GLU:N    | 2.74                     | 0.42              |
| 1:A:264:ARG:HB2  | 1:A:266:TRP:CZ3  | 2.54                     | 0.42              |
| 2:E:13:GLN:HG3   | 2:E:14:MET:N     | 2.34                     | 0.42              |
| 2:F:72:ASP:HA    | 2:F:113:LEU:CD1  | 2.49                     | 0.42              |
| 3:G:372:G:H1     | 5:I:67:U:H3      | 1.67                     | 0.42              |
| 5:I:102:A:H3'    | 5:I:103:A:C8     | 2.54                     | 0.42              |
| 5:I:112:A:C4     | 5:I:123:A:C5     | 3.08                     | 0.42              |
| 1:A:7:ASN:HA     | 5:I:120:U:O2     | 2.19                     | 0.42              |
| 1:A:146:ILE:O    | 1:A:148:ARG:N    | 2.53                     | 0.42              |
| 1:A:187:GLN:HA   | 1:A:313:HIS:CE1  | 2.54                     | 0.42              |
| 1:A:264:ARG:NH1  | 1:A:271:LEU:HB3  | 2.35                     | 0.42              |
| 1:A:264:ARG:NH1  | 1:A:266:TRP:HH2  | 2.17                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:75:LEU:HD22  | 2:B:113:LEU:HD22 | 2.01                     | 0.42              |
| 2:C:35:PRO:HG2   | 2:C:91:PRO:CB    | 2.50                     | 0.42              |
| 2:C:56:PHE:HZ    | 2:C:75:LEU:HD21  | 1.84                     | 0.42              |
| 5:I:26:G:C6      | 5:I:27:G:C5      | 3.08                     | 0.42              |
| 5:I:99:C:N3      | 5:I:132:G:O6     | 2.53                     | 0.42              |
| 1:A:45:ASN:O     | 2:B:1:MET:HE2    | 2.20                     | 0.42              |
| 1:A:271:LEU:HG   | 5:I:86:U:H2'     | 2.01                     | 0.42              |
| 2:C:20:TYR:HA    | 2:C:109:VAL:HG21 | 2.01                     | 0.42              |
| 2:D:28:TYR:CD2   | 2:D:46:LEU:HD22  | 2.55                     | 0.42              |
| 2:E:20:TYR:HH    | 2:E:49:LEU:HA    | 1.85                     | 0.42              |
| 1:A:12:ILE:HG21  | 1:A:167:LEU:CD2  | 2.49                     | 0.42              |
| 1:A:33:TRP:O     | 1:A:37:GLU:HB3   | 2.20                     | 0.42              |
| 1:A:49:LEU:O     | 1:A:50:GLN:C     | 2.63                     | 0.42              |
| 1:A:123:GLN:NE2  | 1:A:269:HIS:O    | 2.52                     | 0.42              |
| 1:A:261:LEU:HD23 | 1:A:261:LEU:HA   | 1.70                     | 0.42              |
| 2:B:53:VAL:HG21  | 2:C:80:PHE:CZ    | 2.55                     | 0.42              |
| 2:E:30:ILE:HG12  | 2:E:98:GLN:NE2   | 2.35                     | 0.42              |
| 2:E:34:ILE:HD13  | 2:E:34:ILE:HG21  | 1.79                     | 0.42              |
| 5:I:9:U:H3       | 5:I:29:G:H1      | 1.68                     | 0.42              |
| 5:I:123:A:H2'    | 5:I:124:A:O4'    | 2.20                     | 0.42              |
| 1:A:29:LYS:CE    | 1:A:321:GLU:HG2  | 2.50                     | 0.42              |
| 1:A:258:ILE:O    | 1:A:264:ARG:HA   | 2.19                     | 0.42              |
| 1:A:263:TYR:HE2  | 4:H:118:U:OP2    | 2.02                     | 0.42              |
| 2:B:7:ALA:HB3    | 2:C:117:ILE:HD13 | 2.02                     | 0.42              |
| 2:F:36:ARG:HB2   | 5:I:5:G:OP1      | 2.20                     | 0.42              |
| 2:F:73:ALA:HA    | 2:F:76:ALA:HB3   | 2.02                     | 0.42              |
| 1:A:159:ILE:HG22 | 1:A:165:ARG:HD3  | 2.01                     | 0.42              |
| 1:A:218:VAL:HG21 | 1:A:260:PHE:HB2  | 2.01                     | 0.42              |
| 1:A:275:SER:HB2  | 5:I:81:A:N1      | 2.35                     | 0.42              |
| 2:B:3:PRO:O      | 2:B:4:ILE:C      | 2.63                     | 0.42              |
| 2:B:32:GLN:HE21  | 2:B:32:GLN:HB3   | 1.40                     | 0.42              |
| 2:B:43:GLU:HA    | 2:C:40:VAL:HG21  | 2.02                     | 0.42              |
| 2:B:68:LEU:HD23  | 2:B:68:LEU:HA    | 1.91                     | 0.42              |
| 2:E:30:ILE:HD13  | 2:E:98:GLN:HB3   | 2.01                     | 0.42              |
| 2:E:90:LYS:O     | 2:E:92:HIS:N     | 2.53                     | 0.42              |
| 1:A:142:PHE:HZ   | 1:A:194:GLY:CA   | 2.33                     | 0.41              |
| 1:A:147:ASP:HB2  | 1:A:193:TYR:CZ   | 2.55                     | 0.41              |
| 1:A:159:ILE:O    | 1:A:160:HIS:CB   | 2.63                     | 0.41              |
| 2:B:13:GLN:HB3   | 2:B:60:GLY:CA    | 2.49                     | 0.41              |
| 2:C:44:MET:HB3   | 2:C:44:MET:HE2   | 1.81                     | 0.41              |
| 2:D:27:LEU:O     | 2:D:31:ALA:N     | 2.44                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:36:ARG:O     | 2:E:38:HIS:N     | 2.53                     | 0.41              |
| 2:E:54:GLU:HB2   | 2:F:77:MET:HE2   | 2.01                     | 0.41              |
| 2:F:16:ILE:HG13  | 2:F:116:TRP:CE3  | 2.55                     | 0.41              |
| 5:I:31:G:H2'     | 5:I:32:C:O4'     | 2.20                     | 0.41              |
| 1:A:146:ILE:HG22 | 1:A:148:ARG:H    | 1.84                     | 0.41              |
| 1:A:308:GLN:HG3  | 1:A:309:TRP:N    | 2.34                     | 0.41              |
| 1:A:315:LEU:O    | 1:A:315:LEU:HD23 | 2.20                     | 0.41              |
| 2:D:35:PRO:O     | 2:D:36:ARG:C     | 2.62                     | 0.41              |
| 2:E:85:LEU:HB3   | 2:E:94:MET:HG3   | 2.01                     | 0.41              |
| 1:A:201:LEU:HG   | 1:A:234:LEU:CD1  | 2.50                     | 0.41              |
| 2:B:88:ILE:HG12  | 2:F:25:SER:HB2   | 2.02                     | 0.41              |
| 2:D:20:TYR:CD2   | 2:D:53:VAL:HG22  | 2.55                     | 0.41              |
| 2:D:45:PHE:CG    | 2:D:85:LEU:HD11  | 2.54                     | 0.41              |
| 2:D:46:LEU:HD23  | 2:D:46:LEU:HA    | 1.75                     | 0.41              |
| 2:F:81:TRP:O     | 2:F:85:LEU:HG    | 2.20                     | 0.41              |
| 1:A:256:ARG:HH11 | 1:A:256:ARG:HB3  | 1.84                     | 0.41              |
| 2:C:26:TYR:O     | 2:C:30:ILE:HG12  | 2.20                     | 0.41              |
| 2:D:56:PHE:CE1   | 2:D:71:ALA:HB1   | 2.55                     | 0.41              |
| 2:D:75:LEU:O     | 2:D:79:ARG:N     | 2.41                     | 0.41              |
| 2:D:77:MET:HE3   | 2:D:81:TRP:NE1   | 2.34                     | 0.41              |
| 2:E:53:VAL:HB    | 2:F:77:MET:HE1   | 2.03                     | 0.41              |
| 2:E:60:GLY:HA2   | 2:E:116:TRP:CZ2  | 2.55                     | 0.41              |
| 2:F:45:PHE:CD2   | 2:F:85:LEU:HD11  | 2.56                     | 0.41              |
| 1:A:141:LYS:HB3  | 1:A:308:GLN:HB2  | 2.02                     | 0.41              |
| 1:A:187:GLN:HA   | 1:A:313:HIS:ND1  | 2.36                     | 0.41              |
| 2:B:44:MET:HE1   | 2:F:47:LYS:HA    | 2.01                     | 0.41              |
| 2:C:45:PHE:CG    | 2:C:85:LEU:HD11  | 2.55                     | 0.41              |
| 2:D:19:ARG:HG3   | 2:D:112:ILE:CD1  | 2.50                     | 0.41              |
| 2:F:20:TYR:OH    | 2:F:49:LEU:HD12  | 2.19                     | 0.41              |
| 1:A:29:LYS:HZ1   | 1:A:321:GLU:HG2  | 1.85                     | 0.41              |
| 2:B:27:LEU:HD23  | 2:B:27:LEU:HA    | 1.83                     | 0.41              |
| 2:B:31:ALA:O     | 2:B:42:ARG:HD3   | 2.21                     | 0.41              |
| 2:C:23:VAL:CG2   | 2:C:109:VAL:HG21 | 2.51                     | 0.41              |
| 2:D:48:CYS:O     | 2:D:52:GLN:HB2   | 2.20                     | 0.41              |
| 2:E:30:ILE:HD13  | 2:E:30:ILE:HG21  | 1.86                     | 0.41              |
| 5:I:105:G:C4     | 5:I:129:G:C2     | 3.09                     | 0.41              |
| 5:I:112:A:C5     | 5:I:123:A:C5     | 3.08                     | 0.41              |
| 1:A:141:LYS:C    | 1:A:144:PRO:HD2  | 2.46                     | 0.41              |
| 2:B:62:SER:O     | 2:B:64:GLN:N     | 2.53                     | 0.41              |
| 2:C:16:ILE:HD13  | 2:C:16:ILE:HA    | 1.77                     | 0.41              |
| 2:D:43:GLU:HA    | 2:E:40:VAL:HG21  | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:82:LEU:HD22  | 2:E:94:MET:HE1   | 2.03                     | 0.41              |
| 2:E:90:LYS:HD3   | 2:E:90:LYS:HA    | 1.29                     | 0.41              |
| 2:E:106:ILE:HA   | 2:E:109:VAL:HG22 | 2.01                     | 0.41              |
| 2:F:44:MET:HE2   | 2:F:44:MET:HB3   | 1.67                     | 0.41              |
| 1:A:57:ASN:HD22  | 1:A:57:ASN:HA    | 1.47                     | 0.41              |
| 2:E:81:TRP:HE3   | 2:E:85:LEU:HD22  | 1.86                     | 0.41              |
| 2:E:99:VAL:O     | 2:E:103:GLN:CG   | 2.69                     | 0.41              |
| 5:I:63:U:H2'     | 5:I:64:C:C6      | 2.55                     | 0.41              |
| 1:A:98:PHE:CE1   | 1:A:158:LYS:CB   | 3.04                     | 0.41              |
| 1:A:304:SER:O    | 1:A:308:GLN:HB3  | 2.21                     | 0.41              |
| 1:A:310:ALA:HB3  | 1:A:312:THR:HG23 | 2.02                     | 0.41              |
| 2:B:43:GLU:HG2   | 2:C:40:VAL:HG22  | 2.02                     | 0.41              |
| 2:C:19:ARG:HD2   | 2:C:108:GLU:CG   | 2.50                     | 0.41              |
| 2:C:39:GLY:HA2   | 2:C:42:ARG:HB3   | 2.03                     | 0.41              |
| 2:D:81:TRP:O     | 2:D:85:LEU:HG    | 2.20                     | 0.41              |
| 2:E:37:LYS:HA    | 2:E:37:LYS:HD2   | 1.74                     | 0.41              |
| 2:F:52:GLN:OE1   | 2:F:74:GLY:C     | 2.63                     | 0.41              |
| 5:I:37:C:H6      | 5:I:37:C:H2'     | 1.70                     | 0.41              |
| 5:I:59:C:H6      | 5:I:60:G:H1'     | 1.85                     | 0.41              |
| 5:I:77:G:H3'     | 5:I:78:C:H6      | 1.85                     | 0.41              |
| 5:I:92:G:H3'     | 5:I:93:G:H4'     | 2.03                     | 0.41              |
| 5:I:132:G:C6     | 5:I:133:C:C4     | 3.09                     | 0.41              |
| 2:D:28:TYR:CE2   | 2:E:41:ALA:HB2   | 2.56                     | 0.41              |
| 2:E:27:LEU:HD23  | 2:E:30:ILE:HD12  | 2.03                     | 0.41              |
| 2:F:30:ILE:HG21  | 2:F:98:GLN:HE22  | 1.85                     | 0.41              |
| 2:F:90:LYS:HB3   | 2:F:91:PRO:HD2   | 2.03                     | 0.41              |
| 2:F:97:HIS:NE2   | 2:F:101:THR:HG21 | 2.36                     | 0.41              |
| 1:A:135:LEU:HD23 | 1:A:219:VAL:HB   | 2.03                     | 0.40              |
| 1:A:213:TYR:C    | 1:A:311:ASP:OD2  | 2.65                     | 0.40              |
| 2:C:108:GLU:O    | 2:C:112:ILE:HG13 | 2.21                     | 0.40              |
| 5:I:116:A:H2'    | 5:I:117:A:O4'    | 2.21                     | 0.40              |
| 1:A:152:TYR:HE2  | 1:A:172:LEU:HD23 | 1.85                     | 0.40              |
| 1:A:260:PHE:CE2  | 1:A:261:LEU:HD12 | 2.56                     | 0.40              |
| 2:C:20:TYR:CG    | 2:C:56:PHE:HE2   | 2.39                     | 0.40              |
| 2:E:32:GLN:OE1   | 2:F:37:LYS:O     | 2.39                     | 0.40              |
| 2:C:38:HIS:HE1   | 2:C:90:LYS:CD    | 2.30                     | 0.40              |
| 2:D:28:TYR:CE1   | 2:D:32:GLN:CG    | 3.04                     | 0.40              |
| 2:D:34:ILE:HG22  | 2:D:38:HIS:HB2   | 2.04                     | 0.40              |
| 2:E:57:ILE:HD13  | 2:F:77:MET:HA    | 2.02                     | 0.40              |
| 1:A:19:LEU:O     | 1:A:22:TYR:N     | 2.55                     | 0.40              |
| 1:A:116:HIS:O    | 1:A:119:VAL:HG22 | 2.22                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:C:71:ALA:C    | 2:C:113:LEU:HD21 | 2.47                     | 0.40              |
| 2:E:36:ARG:C    | 2:E:38:HIS:N     | 2.78                     | 0.40              |
| 2:F:94:MET:CG   | 2:F:98:GLN:HB2   | 2.52                     | 0.40              |
| 5:I:121:G:C6    | 5:I:122:G:C4     | 3.09                     | 0.40              |
| 1:A:307:ALA:HB1 | 1:A:312:THR:HG21 | 2.03                     | 0.40              |
| 2:B:46:LEU:HA   | 2:B:46:LEU:HD23  | 1.77                     | 0.40              |
| 2:C:88:ILE:HG22 | 2:C:90:LYS:O     | 2.21                     | 0.40              |
| 2:D:23:VAL:HG12 | 2:D:27:LEU:HD12  | 2.04                     | 0.40              |
| 2:D:72:ASP:N    | 2:D:113:LEU:HD21 | 2.37                     | 0.40              |
| 2:E:20:TYR:CE2  | 2:E:49:LEU:O     | 2.75                     | 0.40              |
| 2:E:60:GLY:C    | 2:E:62:SER:N     | 2.80                     | 0.40              |
| 2:E:102:ALA:HA  | 2:E:105:LEU:HD12 | 2.04                     | 0.40              |
| 2:F:82:LEU:HD22 | 2:F:94:MET:SD    | 2.62                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |           |
|-----|-------|----------------|-----------|----------|----------|-------------|-----------|
| 1   | A     | 309/328 (94%)  | 228 (74%) | 63 (20%) | 18 (6%)  | <b>1</b>    | <b>6</b>  |
| 2   | B     | 120/290 (41%)  | 108 (90%) | 8 (7%)   | 4 (3%)   | <b>3</b>    | <b>13</b> |
| 2   | C     | 109/290 (38%)  | 99 (91%)  | 3 (3%)   | 7 (6%)   | <b>1</b>    | <b>5</b>  |
| 2   | D     | 108/290 (37%)  | 97 (90%)  | 10 (9%)  | 1 (1%)   | <b>14</b>   | <b>39</b> |
| 2   | E     | 108/290 (37%)  | 97 (90%)  | 8 (7%)   | 3 (3%)   | <b>4</b>    | <b>16</b> |
| 2   | F     | 108/290 (37%)  | 100 (93%) | 7 (6%)   | 1 (1%)   | <b>14</b>   | <b>39</b> |
| All | All   | 862/1778 (48%) | 729 (85%) | 99 (12%) | 34 (4%)  | <b>4</b>    | <b>11</b> |

All (34) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | ASN  |
| 1   | A     | 109 | CYS  |
| 1   | A     | 138 | ASP  |
| 1   | A     | 214 | MET  |
| 1   | A     | 255 | SER  |
| 2   | C     | 86  | ALA  |
| 2   | C     | 88  | ILE  |
| 2   | C     | 89  | GLN  |
| 2   | C     | 91  | PRO  |
| 2   | C     | 93  | ALA  |
| 1   | A     | 139 | PHE  |
| 1   | A     | 141 | LYS  |
| 1   | A     | 149 | ALA  |
| 1   | A     | 163 | ALA  |
| 1   | A     | 222 | ASP  |
| 2   | B     | 4   | ILE  |
| 2   | B     | 92  | HIS  |
| 2   | E     | 65  | VAL  |
| 1   | A     | 187 | GLN  |
| 1   | A     | 269 | HIS  |
| 2   | B     | 35  | PRO  |
| 2   | D     | 92  | HIS  |
| 2   | E     | 89  | GLN  |
| 1   | A     | 4   | ARG  |
| 1   | A     | 140 | SER  |
| 1   | A     | 186 | SER  |
| 2   | C     | 12  | ASP  |
| 1   | A     | 40  | GLU  |
| 1   | A     | 103 | LEU  |
| 1   | A     | 193 | TYR  |
| 2   | B     | 2   | GLU  |
| 2   | F     | 90  | LYS  |
| 2   | C     | 92  | HIS  |
| 2   | E     | 91  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |   |
|-----|-------|----------------|-----------|-----------|-------------|---|
| 1   | A     | 264/278 (95%)  | 192 (73%) | 72 (27%)  | 0           | 1 |
| 2   | B     | 102/232 (44%)  | 82 (80%)  | 20 (20%)  | 1           | 5 |
| 2   | C     | 92/232 (40%)   | 77 (84%)  | 15 (16%)  | 2           | 9 |
| 2   | D     | 91/232 (39%)   | 73 (80%)  | 18 (20%)  | 1           | 5 |
| 2   | E     | 91/232 (39%)   | 72 (79%)  | 19 (21%)  | 1           | 4 |
| 2   | F     | 91/232 (39%)   | 65 (71%)  | 26 (29%)  | 0           | 1 |
| All | All   | 731/1438 (51%) | 561 (77%) | 170 (23%) | 2           | 3 |

All (170) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | LYS  |
| 1   | A     | 16  | GLU  |
| 1   | A     | 18  | LEU  |
| 1   | A     | 23  | ARG  |
| 1   | A     | 31  | ARG  |
| 1   | A     | 37  | GLU  |
| 1   | A     | 39  | LYS  |
| 1   | A     | 54  | LYS  |
| 1   | A     | 57  | ASN  |
| 1   | A     | 59  | GLU  |
| 1   | A     | 82  | LYS  |
| 1   | A     | 93  | ILE  |
| 1   | A     | 94  | VAL  |
| 1   | A     | 97  | ILE  |
| 1   | A     | 103 | LEU  |
| 1   | A     | 110 | ARG  |
| 1   | A     | 115 | THR  |
| 1   | A     | 119 | VAL  |
| 1   | A     | 127 | ARG  |
| 1   | A     | 129 | THR  |
| 1   | A     | 130 | ARG  |
| 1   | A     | 132 | THR  |
| 1   | A     | 135 | LEU  |
| 1   | A     | 136 | LYS  |
| 1   | A     | 138 | ASP  |
| 1   | A     | 141 | LYS  |
| 1   | A     | 147 | ASP  |
| 1   | A     | 156 | ASP  |
| 1   | A     | 158 | LYS  |
| 1   | A     | 159 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 161 | CYS  |
| 1   | A     | 165 | ARG  |
| 1   | A     | 171 | VAL  |
| 1   | A     | 172 | LEU  |
| 1   | A     | 175 | GLU  |
| 1   | A     | 177 | VAL  |
| 1   | A     | 179 | ILE  |
| 1   | A     | 181 | ILE  |
| 1   | A     | 184 | LEU  |
| 1   | A     | 187 | GLN  |
| 1   | A     | 197 | VAL  |
| 1   | A     | 200 | LEU  |
| 1   | A     | 204 | GLU  |
| 1   | A     | 208 | ARG  |
| 1   | A     | 215 | ASP  |
| 1   | A     | 217 | ILE  |
| 1   | A     | 225 | GLU  |
| 1   | A     | 226 | GLU  |
| 1   | A     | 227 | LEU  |
| 1   | A     | 240 | GLU  |
| 1   | A     | 244 | LEU  |
| 1   | A     | 246 | ILE  |
| 1   | A     | 247 | SER  |
| 1   | A     | 256 | ARG  |
| 1   | A     | 264 | ARG  |
| 1   | A     | 265 | ILE  |
| 1   | A     | 270 | LYS  |
| 1   | A     | 271 | LEU  |
| 1   | A     | 272 | LEU  |
| 1   | A     | 274 | LYS  |
| 1   | A     | 276 | SER  |
| 1   | A     | 279 | ARG  |
| 1   | A     | 282 | ARG  |
| 1   | A     | 283 | LYS  |
| 1   | A     | 290 | HIS  |
| 1   | A     | 293 | ASP  |
| 1   | A     | 296 | LEU  |
| 1   | A     | 298 | ARG  |
| 1   | A     | 302 | SER  |
| 1   | A     | 317 | THR  |
| 1   | A     | 325 | ILE  |
| 1   | A     | 327 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 8   | THR  |
| 2   | B     | 13  | GLN  |
| 2   | B     | 19  | ARG  |
| 2   | B     | 32  | GLN  |
| 2   | B     | 37  | LYS  |
| 2   | B     | 54  | GLU  |
| 2   | B     | 62  | SER  |
| 2   | B     | 64  | GLN  |
| 2   | B     | 65  | VAL  |
| 2   | B     | 66  | SER  |
| 2   | B     | 67  | LYS  |
| 2   | B     | 75  | LEU  |
| 2   | B     | 85  | LEU  |
| 2   | B     | 89  | GLN  |
| 2   | B     | 90  | LYS  |
| 2   | B     | 97  | HIS  |
| 2   | B     | 100 | GLU  |
| 2   | B     | 108 | GLU  |
| 2   | B     | 115 | SER  |
| 2   | B     | 119 | ARG  |
| 2   | C     | 14  | MET  |
| 2   | C     | 16  | ILE  |
| 2   | C     | 36  | ARG  |
| 2   | C     | 43  | GLU  |
| 2   | C     | 61  | LYS  |
| 2   | C     | 63  | ASN  |
| 2   | C     | 66  | SER  |
| 2   | C     | 68  | LEU  |
| 2   | C     | 85  | LEU  |
| 2   | C     | 88  | ILE  |
| 2   | C     | 90  | LYS  |
| 2   | C     | 91  | PRO  |
| 2   | C     | 92  | HIS  |
| 2   | C     | 94  | MET  |
| 2   | C     | 101 | THR  |
| 2   | D     | 14  | MET  |
| 2   | D     | 15  | LEU  |
| 2   | D     | 18  | GLU  |
| 2   | D     | 36  | ARG  |
| 2   | D     | 37  | LYS  |
| 2   | D     | 52  | GLN  |
| 2   | D     | 58  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 62  | SER  |
| 2   | D     | 63  | ASN  |
| 2   | D     | 64  | GLN  |
| 2   | D     | 65  | VAL  |
| 2   | D     | 68  | LEU  |
| 2   | D     | 89  | GLN  |
| 2   | D     | 95  | THR  |
| 2   | D     | 101 | THR  |
| 2   | D     | 103 | GLN  |
| 2   | D     | 119 | ARG  |
| 2   | D     | 122 | ARG  |
| 2   | E     | 13  | GLN  |
| 2   | E     | 16  | ILE  |
| 2   | E     | 18  | GLU  |
| 2   | E     | 43  | GLU  |
| 2   | E     | 50  | LEU  |
| 2   | E     | 52  | GLN  |
| 2   | E     | 57  | ILE  |
| 2   | E     | 63  | ASN  |
| 2   | E     | 65  | VAL  |
| 2   | E     | 67  | LYS  |
| 2   | E     | 75  | LEU  |
| 2   | E     | 83  | ARG  |
| 2   | E     | 85  | LEU  |
| 2   | E     | 88  | ILE  |
| 2   | E     | 89  | GLN  |
| 2   | E     | 90  | LYS  |
| 2   | E     | 95  | THR  |
| 2   | E     | 113 | LEU  |
| 2   | E     | 119 | ARG  |
| 2   | F     | 13  | GLN  |
| 2   | F     | 14  | MET  |
| 2   | F     | 15  | LEU  |
| 2   | F     | 16  | ILE  |
| 2   | F     | 22  | ARG  |
| 2   | F     | 27  | LEU  |
| 2   | F     | 30  | ILE  |
| 2   | F     | 33  | SER  |
| 2   | F     | 36  | ARG  |
| 2   | F     | 43  | GLU  |
| 2   | F     | 54  | GLU  |
| 2   | F     | 55  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 61  | LYS  |
| 2   | F     | 62  | SER  |
| 2   | F     | 65  | VAL  |
| 2   | F     | 66  | SER  |
| 2   | F     | 83  | ARG  |
| 2   | F     | 88  | ILE  |
| 2   | F     | 90  | LYS  |
| 2   | F     | 95  | THR  |
| 2   | F     | 100 | GLU  |
| 2   | F     | 103 | GLN  |
| 2   | F     | 105 | LEU  |
| 2   | F     | 111 | ARG  |
| 2   | F     | 113 | LEU  |
| 2   | F     | 122 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 57  | ASN  |
| 1   | A     | 121 | HIS  |
| 1   | A     | 187 | GLN  |
| 1   | A     | 259 | ASN  |
| 1   | A     | 286 | ASN  |
| 1   | A     | 290 | HIS  |
| 1   | A     | 314 | ASN  |
| 2   | B     | 13  | GLN  |
| 2   | B     | 89  | GLN  |
| 2   | C     | 13  | GLN  |
| 2   | C     | 32  | GLN  |
| 2   | C     | 89  | GLN  |
| 2   | C     | 92  | HIS  |
| 2   | C     | 97  | HIS  |
| 2   | C     | 121 | ASN  |
| 2   | D     | 13  | GLN  |
| 2   | D     | 32  | GLN  |
| 2   | D     | 52  | GLN  |
| 2   | E     | 13  | GLN  |
| 2   | E     | 97  | HIS  |
| 2   | F     | 92  | HIS  |
| 2   | F     | 97  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed      | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 3   | G     | 10/19 (52%)   | 6 (60%)           | 1 (10%)         |
| 4   | H     | 16/36 (44%)   | 14 (87%)          | 2 (12%)         |
| 5   | I     | 138/140 (98%) | 84 (60%)          | 11 (7%)         |
| All | All   | 164/195 (84%) | 104 (63%)         | 14 (8%)         |

All (104) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | G     | 372 | G    |
| 3   | G     | 373 | C    |
| 3   | G     | 377 | C    |
| 3   | G     | 378 | U    |
| 3   | G     | 379 | G    |
| 3   | G     | 381 | G    |
| 4   | H     | 119 | G    |
| 4   | H     | 120 | C    |
| 4   | H     | 121 | C    |
| 4   | H     | 122 | C    |
| 4   | H     | 125 | C    |
| 4   | H     | 126 | A    |
| 4   | H     | 127 | C    |
| 4   | H     | 128 | C    |
| 4   | H     | 129 | U    |
| 4   | H     | 130 | U    |
| 4   | H     | 131 | C    |
| 4   | H     | 132 | U    |
| 4   | H     | 133 | U    |
| 4   | H     | 134 | G    |
| 5   | I     | 2   | A    |
| 5   | I     | 3   | U    |
| 5   | I     | 4   | G    |
| 5   | I     | 5   | G    |
| 5   | I     | 6   | C    |
| 5   | I     | 7   | U    |
| 5   | I     | 8   | C    |
| 5   | I     | 9   | U    |
| 5   | I     | 11  | C    |
| 5   | I     | 13  | A    |
| 5   | I     | 14  | A    |
| 5   | I     | 15  | C    |
| 5   | I     | 20  | C    |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | I     | 21  | G    |
| 5   | I     | 22  | G    |
| 5   | I     | 25  | U    |
| 5   | I     | 27  | G    |
| 5   | I     | 28  | C    |
| 5   | I     | 29  | G    |
| 5   | I     | 31  | G    |
| 5   | I     | 34  | G    |
| 5   | I     | 35  | G    |
| 5   | I     | 36  | C    |
| 5   | I     | 37  | C    |
| 5   | I     | 39  | U    |
| 5   | I     | 40  | U    |
| 5   | I     | 41  | C    |
| 5   | I     | 42  | C    |
| 5   | I     | 43  | U    |
| 5   | I     | 47  | U    |
| 5   | I     | 49  | G    |
| 5   | I     | 52  | G    |
| 5   | I     | 55  | C    |
| 5   | I     | 56  | A    |
| 5   | I     | 57  | G    |
| 5   | I     | 58  | C    |
| 5   | I     | 59  | C    |
| 5   | I     | 60  | G    |
| 5   | I     | 61  | G    |
| 5   | I     | 62  | U    |
| 5   | I     | 63  | U    |
| 5   | I     | 64  | C    |
| 5   | I     | 65  | U    |
| 5   | I     | 66  | G    |
| 5   | I     | 71  | G    |
| 5   | I     | 73  | U    |
| 5   | I     | 74  | U    |
| 5   | I     | 75  | C    |
| 5   | I     | 76  | G    |
| 5   | I     | 77  | G    |
| 5   | I     | 78  | C    |
| 5   | I     | 79  | G    |
| 5   | I     | 80  | A    |
| 5   | I     | 81  | A    |
| 5   | I     | 82  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | I     | 83  | A    |
| 5   | I     | 84  | C    |
| 5   | I     | 85  | G    |
| 5   | I     | 86  | U    |
| 5   | I     | 87  | U    |
| 5   | I     | 88  | A    |
| 5   | I     | 89  | C    |
| 5   | I     | 90  | A    |
| 5   | I     | 91  | C    |
| 5   | I     | 92  | G    |
| 5   | I     | 93  | G    |
| 5   | I     | 94  | U    |
| 5   | I     | 95  | U    |
| 5   | I     | 97  | G    |
| 5   | I     | 98  | G    |
| 5   | I     | 99  | C    |
| 5   | I     | 101 | A    |
| 5   | I     | 106 | U    |
| 5   | I     | 109 | A    |
| 5   | I     | 110 | U    |
| 5   | I     | 118 | A    |
| 5   | I     | 119 | A    |
| 5   | I     | 120 | U    |
| 5   | I     | 125 | A    |
| 5   | I     | 126 | G    |
| 5   | I     | 129 | G    |
| 5   | I     | 130 | G    |
| 5   | I     | 131 | G    |
| 5   | I     | 132 | G    |

All (14) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | G     | 380 | G    |
| 4   | H     | 127 | C    |
| 4   | H     | 129 | U    |
| 5   | I     | 7   | U    |
| 5   | I     | 20  | C    |
| 5   | I     | 27  | G    |
| 5   | I     | 42  | C    |
| 5   | I     | 63  | U    |
| 5   | I     | 74  | U    |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | I     | 81  | A    |
| 5   | I     | 88  | A    |
| 5   | I     | 91  | C    |
| 5   | I     | 94  | U    |
| 5   | I     | 100 | A    |

## 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](#)

There are no chain breaks in this entry.

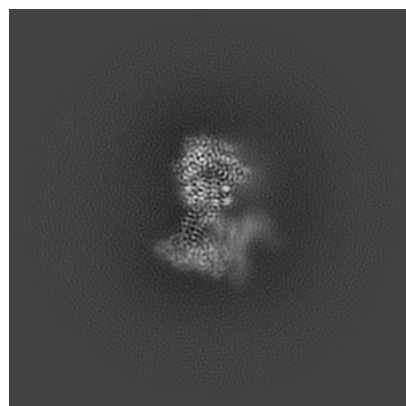
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42084. These allow visual inspection of the internal detail of the map and identification of artifacts.

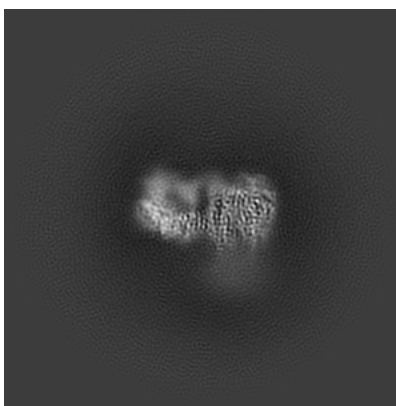
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

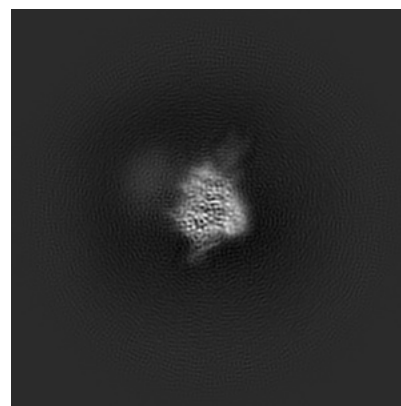
#### 6.1.1 Primary map



X

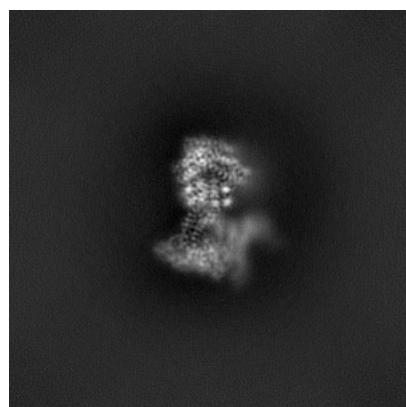


Y

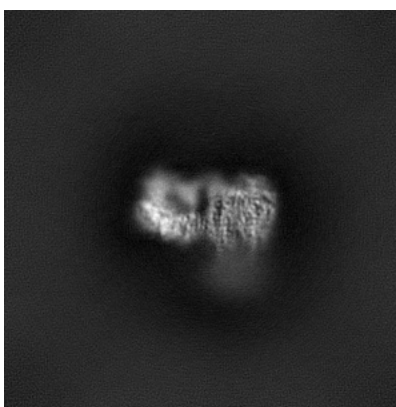


Z

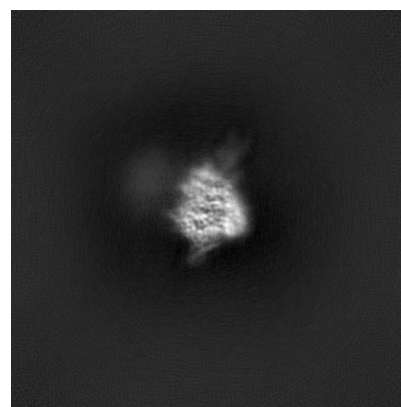
#### 6.1.2 Raw map



X



Y



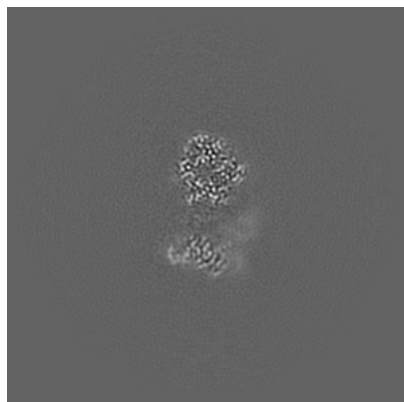
Z

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

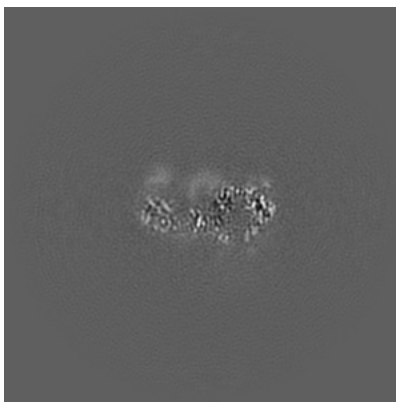


## 6.2 Central slices [i](#)

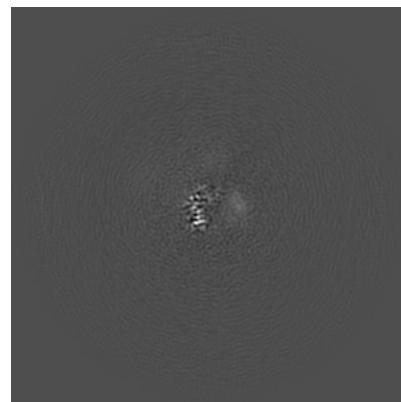
### 6.2.1 Primary map



X Index: 160

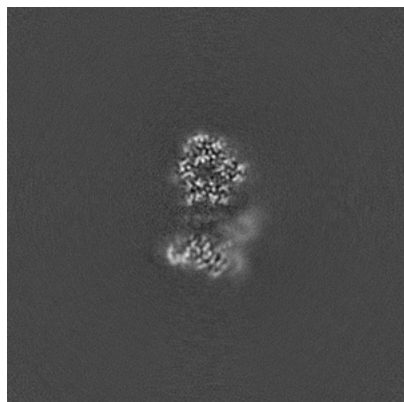


Y Index: 160

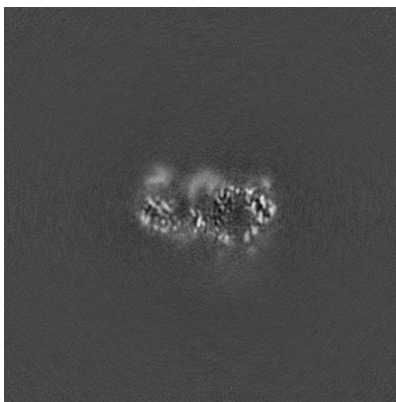


Z Index: 160

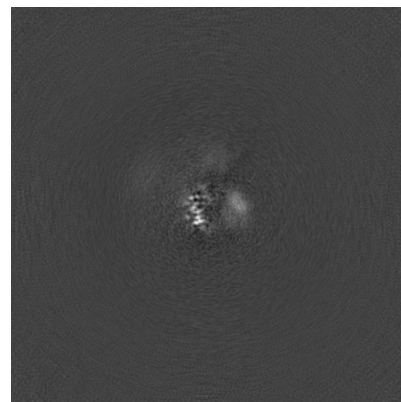
### 6.2.2 Raw map



X Index: 160



Y Index: 160

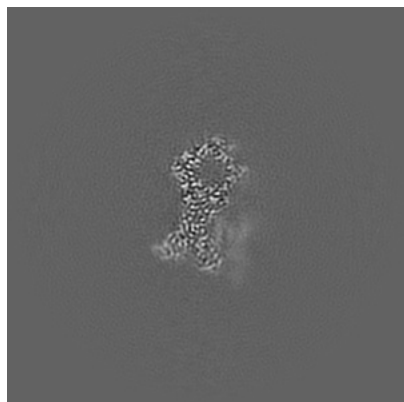


Z Index: 160

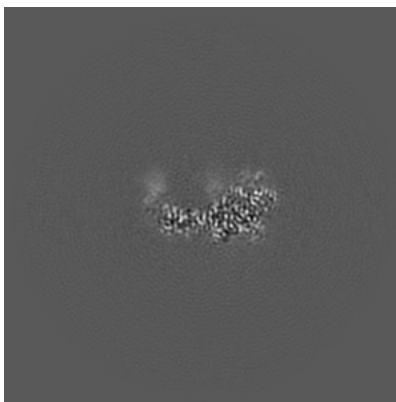
The images above show central slices of the map in three orthogonal directions.

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

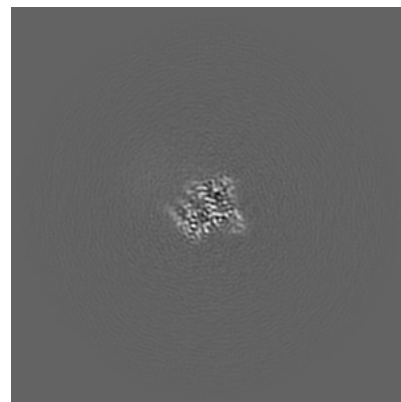
### 6.3.1 Primary map



X Index: 151

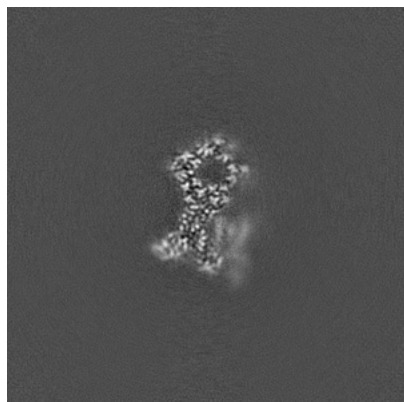


Y Index: 148

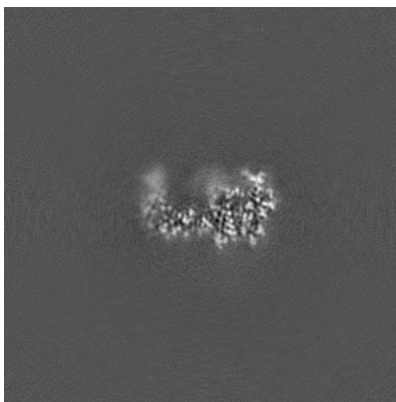


Z Index: 199

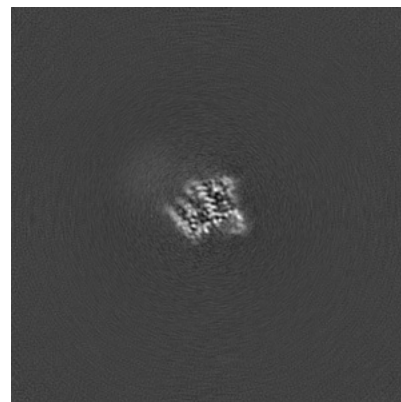
### 6.3.2 Raw map



X Index: 150



Y Index: 151

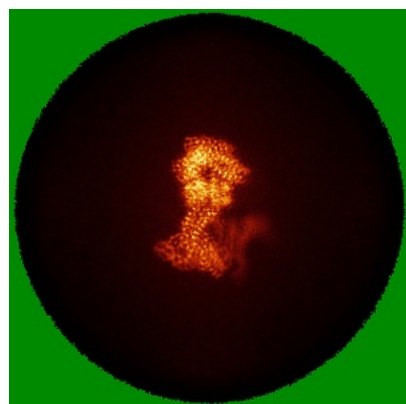


Z Index: 199

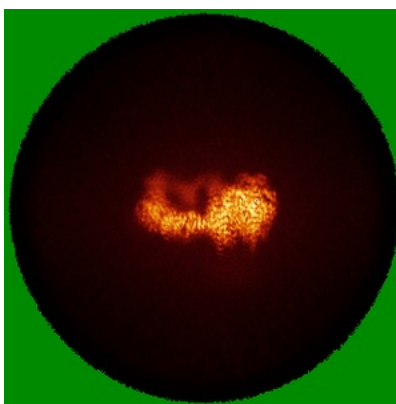
The images above show the largest variance slices of the map in three orthogonal directions.

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

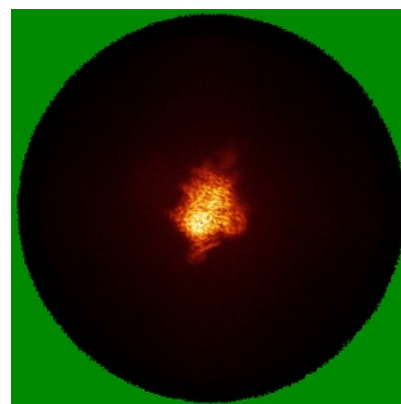
### 6.4.1 Primary map



X

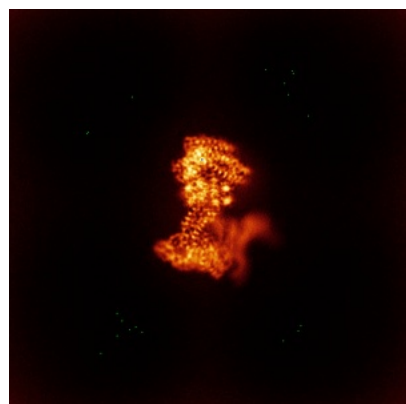


Y

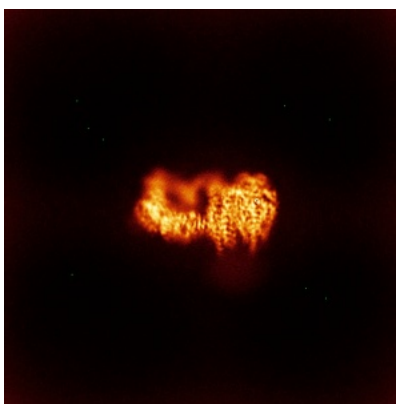


Z

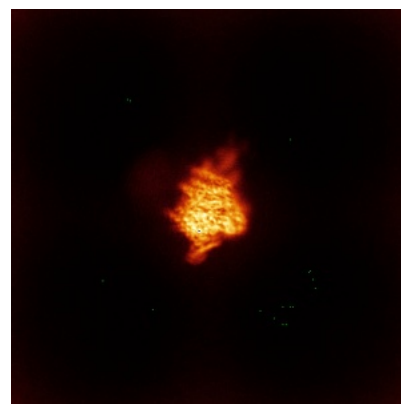
### 6.4.2 Raw map



X



Y

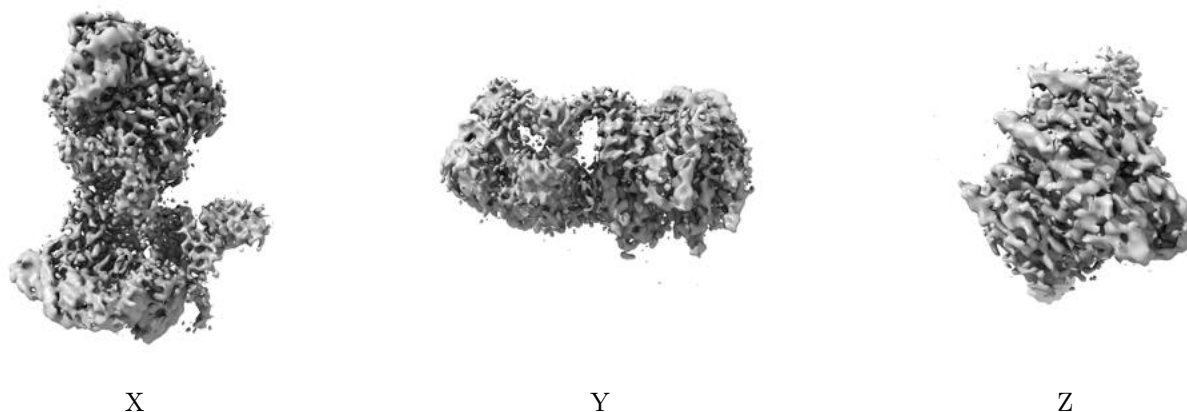


Z

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 0.2. 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.

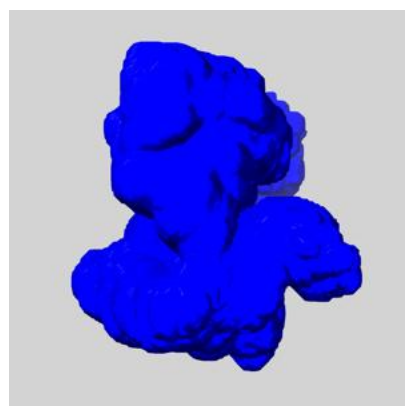
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

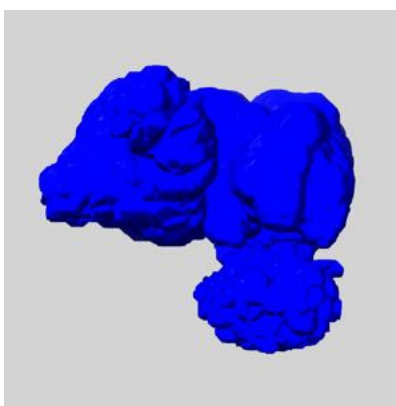
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

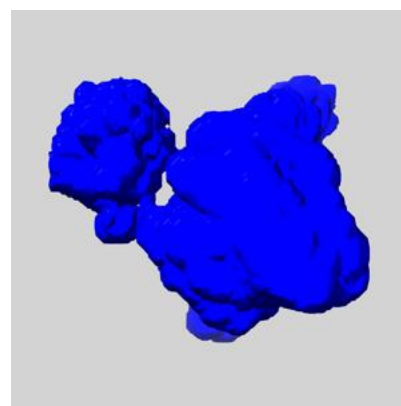
### 6.6.1 emd\_42084\_msk\_1.map [i](#)



X



Y

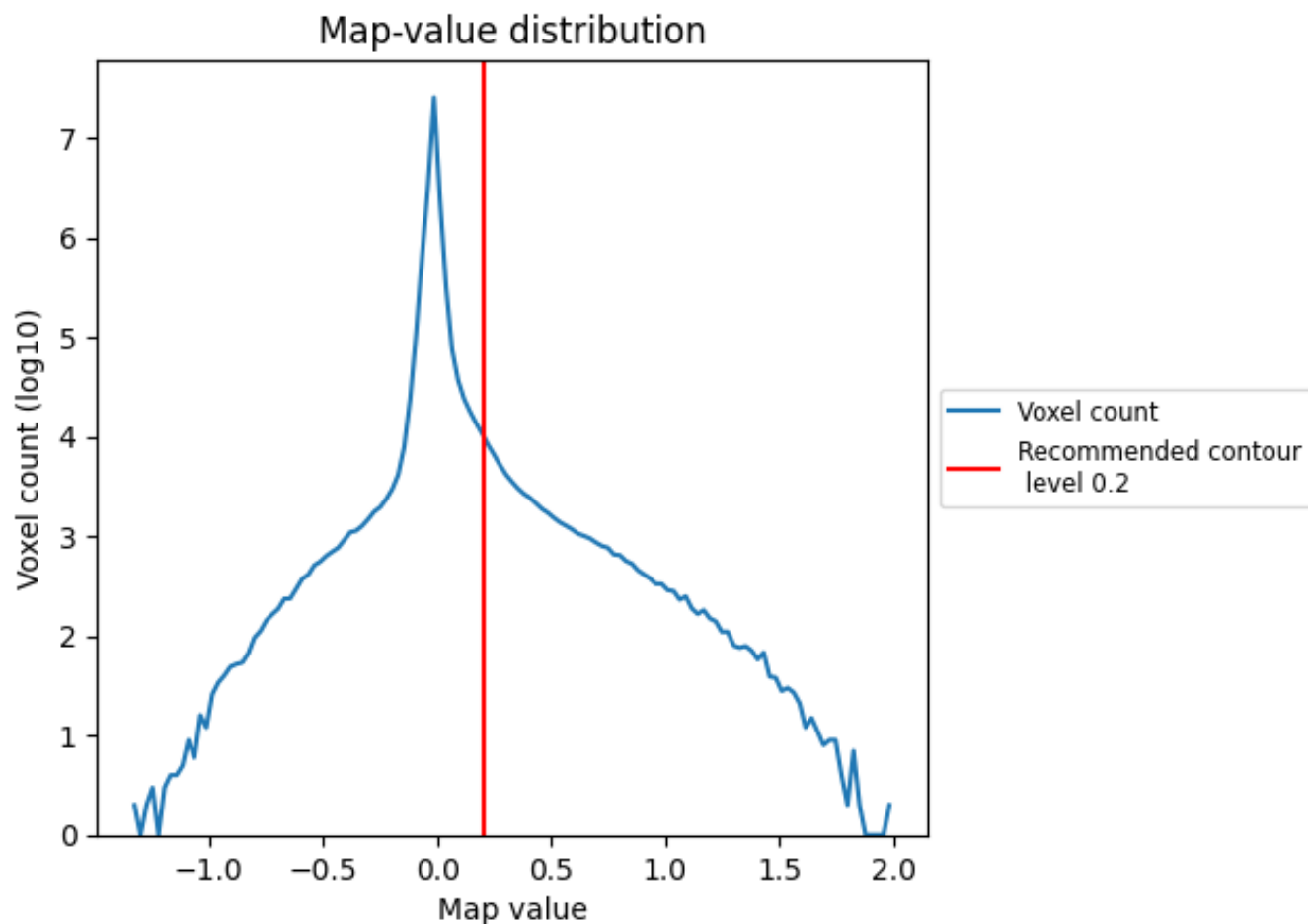


Z

## 7 Map analysis [i](#)

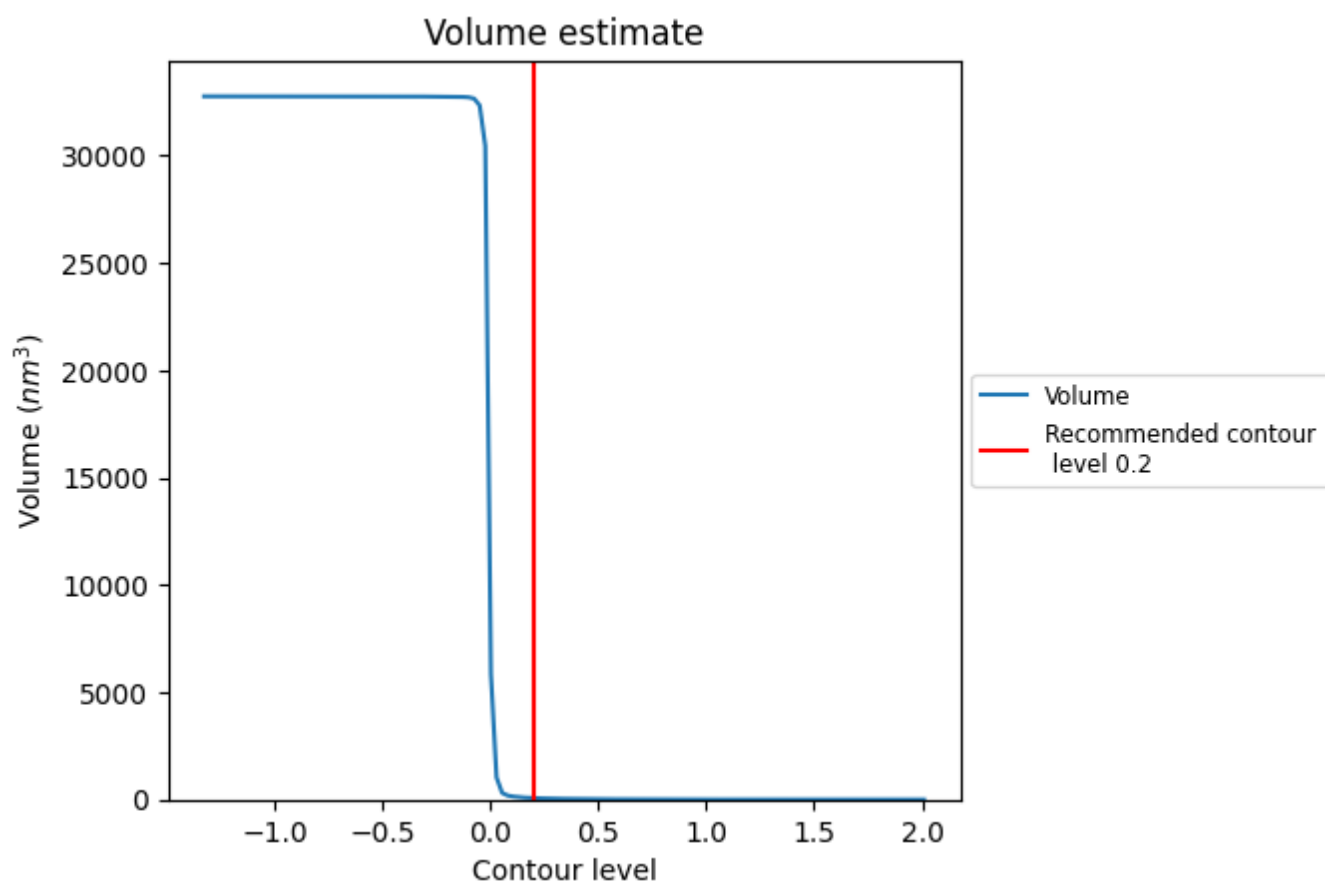
This section contains the results of statistical analysis of the map.

### 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.

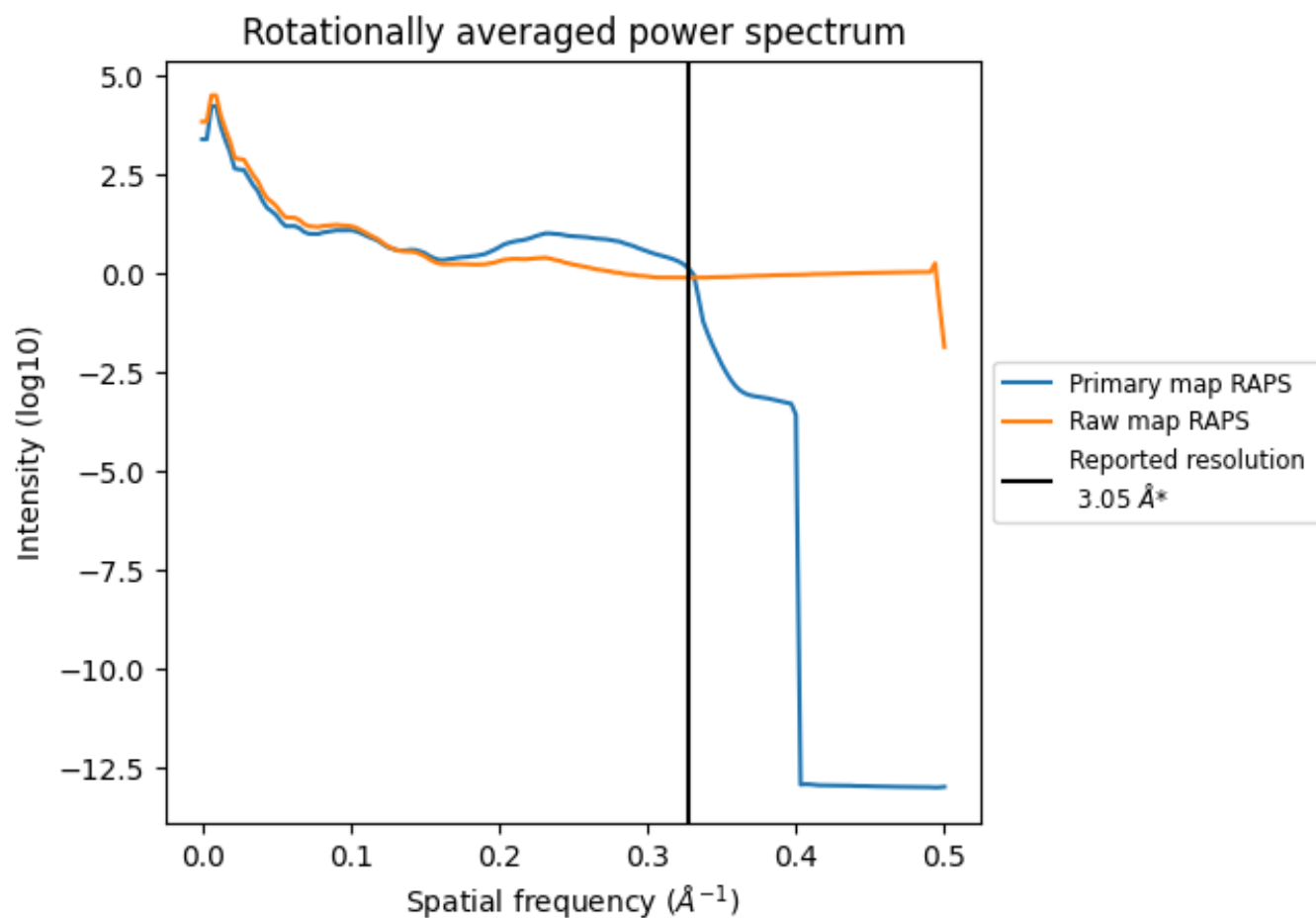
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 69 nm<sup>3</sup>; this corresponds to an approximate mass of 63 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 ⓘ



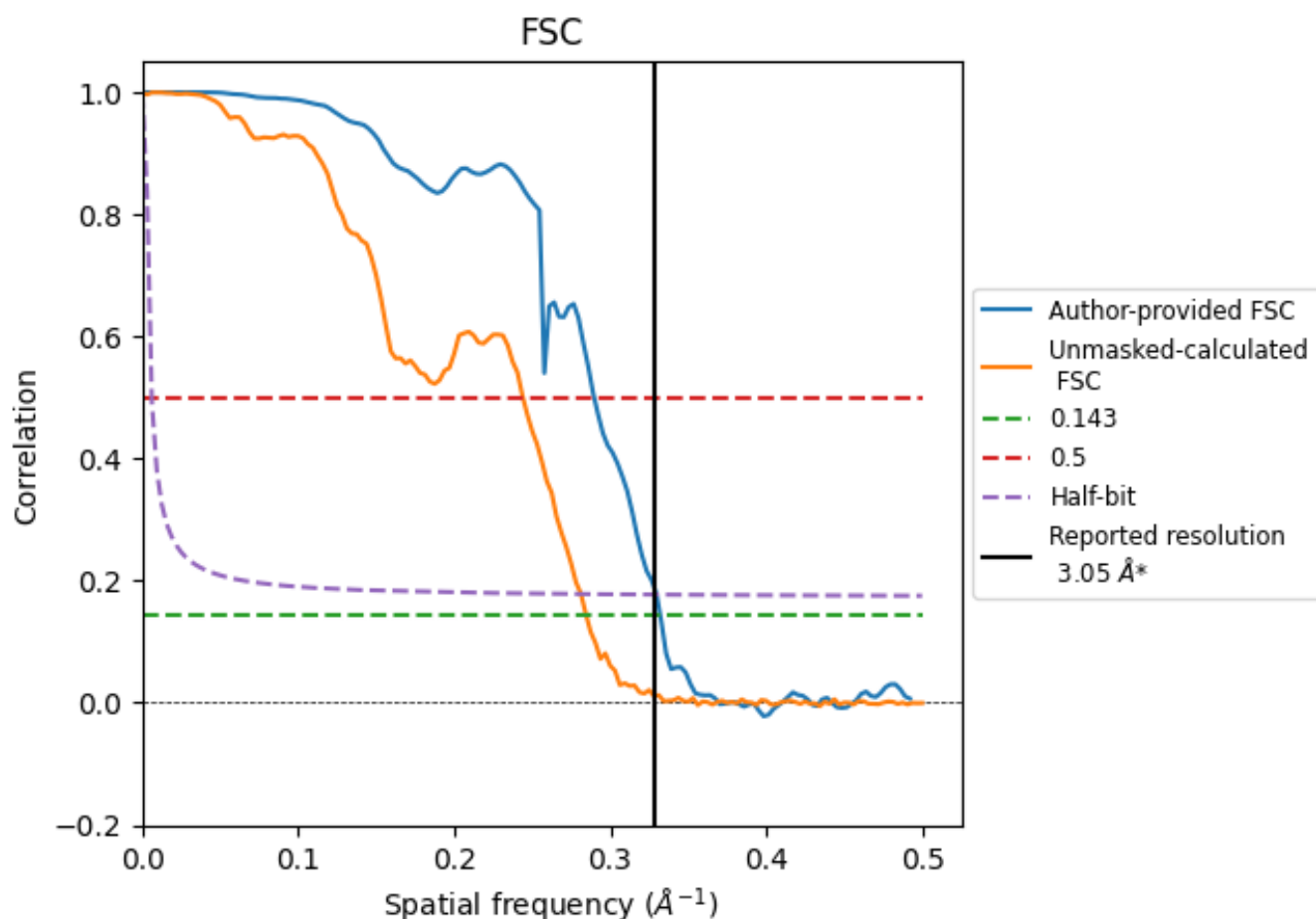
\*Reported resolution corresponds to spatial frequency of 0.328 Å<sup>-1</sup>



## 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 0.328  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

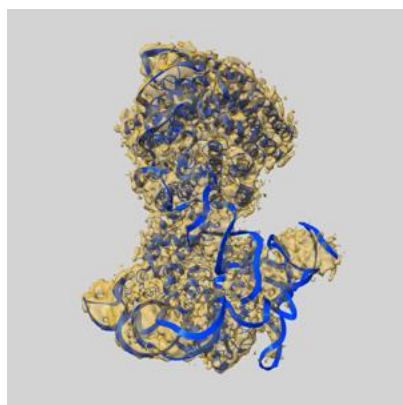
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.05                               | -    | -        |
| Author-provided FSC curve | 3.01                               | 3.45 | 3.03     |
| Unmasked-calculated*      | 3.51                               | 4.10 | 3.55     |

\*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 3.51 differs from the reported value 3.05 by more than 10 %

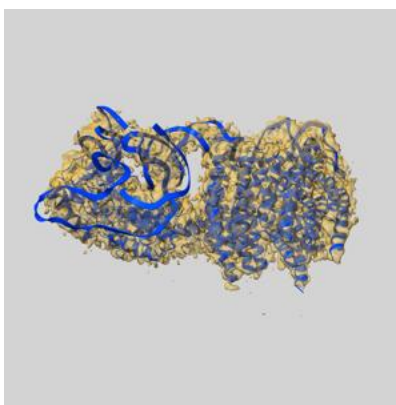
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42084 and PDB model 8UBE. Per-residue inclusion information can be found in section 3 on page 6.

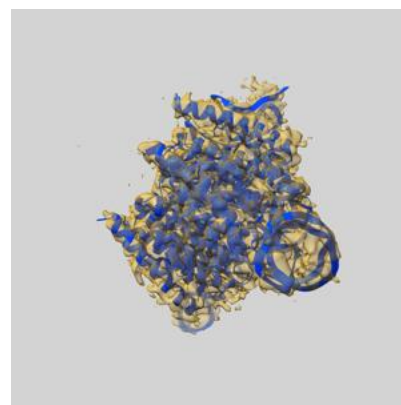
### 9.1 Map-model overlay [i](#)



X



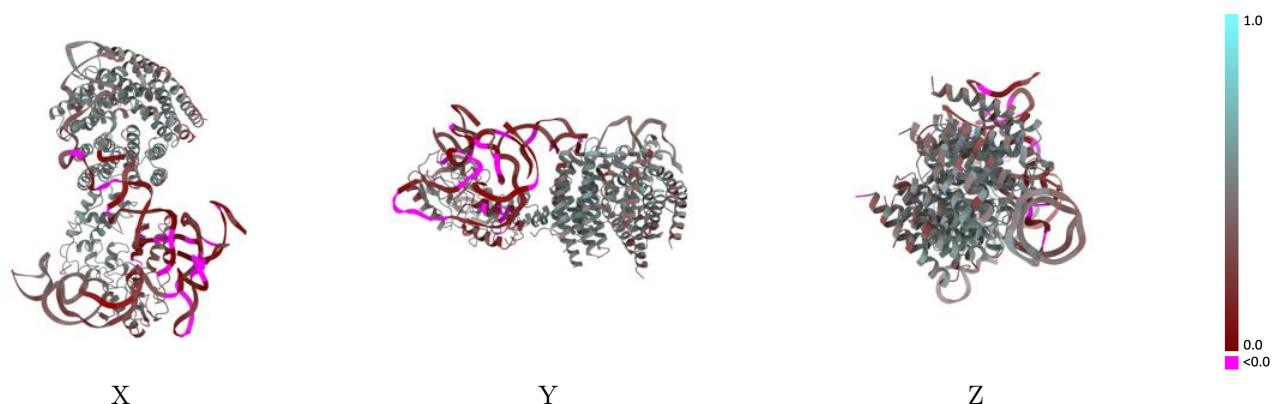
Y



Z

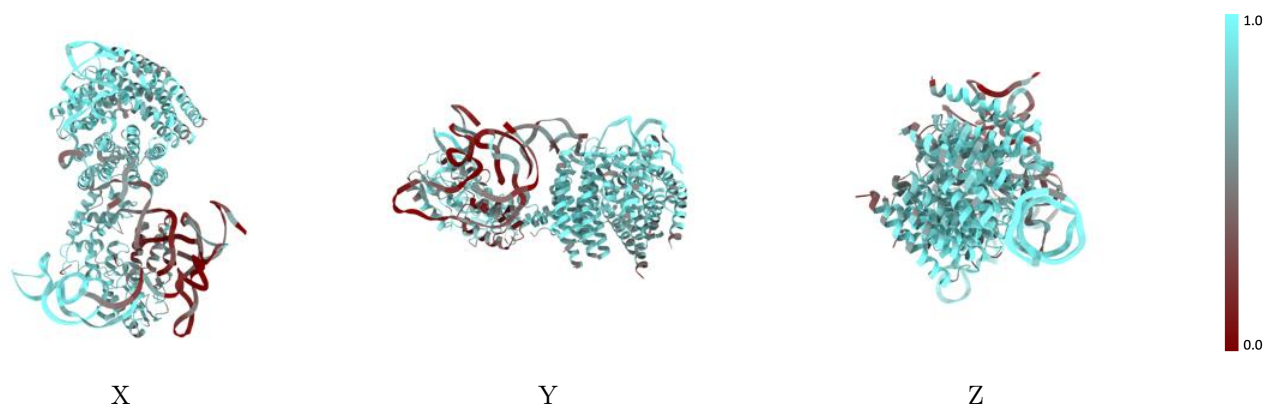
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



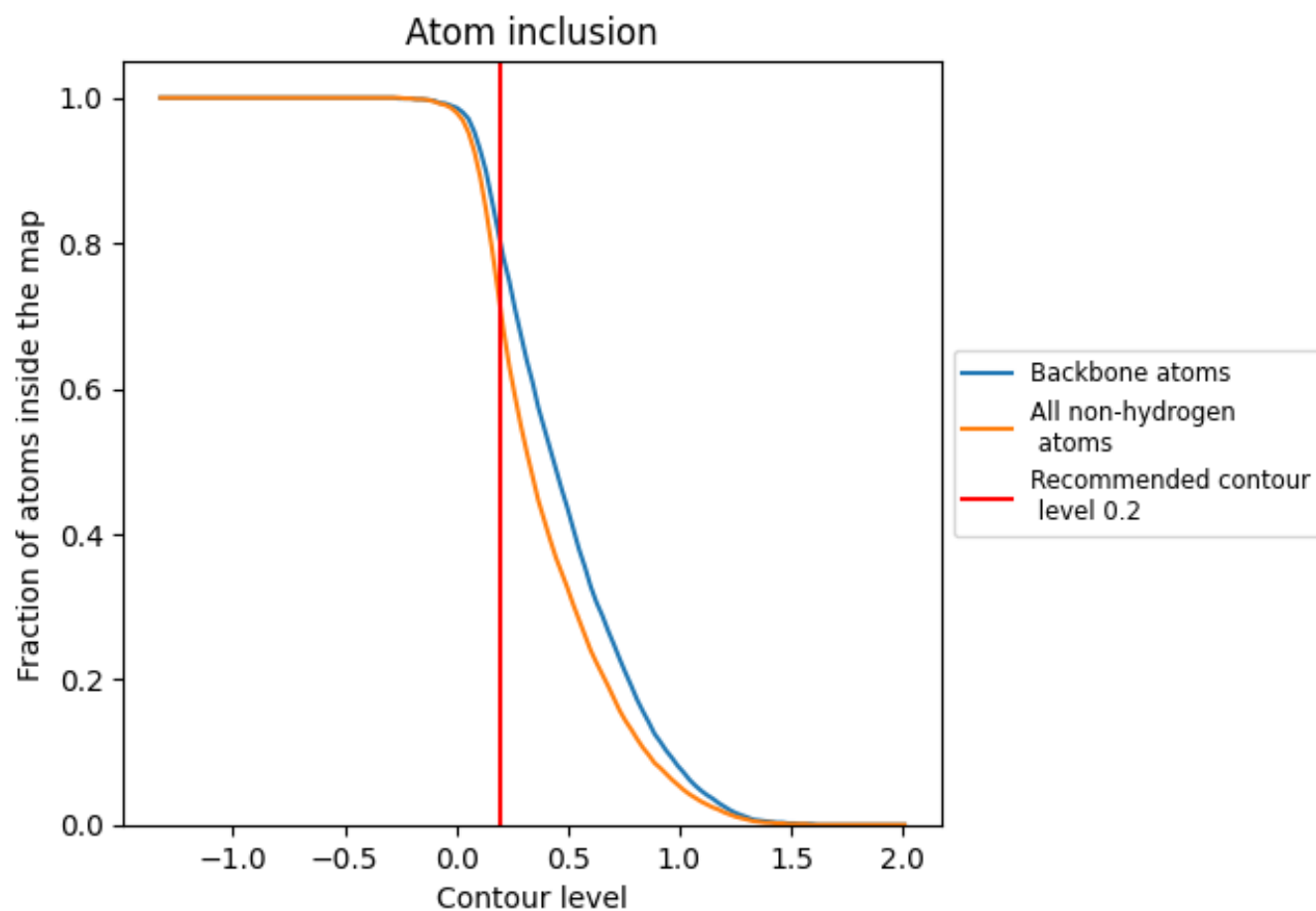
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 71% 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 (0.2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.7060 | <div></div> 0.3700 |
| A     | <div></div> 0.6960 | <div></div> 0.3980 |
| B     | <div></div> 0.8370 | <div></div> 0.4950 |
| C     | <div></div> 0.8600 | <div></div> 0.4930 |
| D     | <div></div> 0.8220 | <div></div> 0.4570 |
| E     | <div></div> 0.8160 | <div></div> 0.4650 |
| F     | <div></div> 0.8300 | <div></div> 0.4690 |
| G     | <div></div> 0.3290 | <div></div> 0.0680 |
| H     | <div></div> 0.3230 | <div></div> 0.0880 |
| I     | <div></div> 0.6030 | <div></div> 0.2440 |

1.0

0.0

<0.0