



## Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 03:46 AM UTC

PDB ID : 9NO1 / pdb\_00009no1  
EMDB ID : EMD-49591  
Title : Cryo-ET map of the VZV capsid vertex (5-fold axis).  
Authors : Oliver, S.L.; Chen, M.  
Deposited on : 2025-03-07  
Resolution : 8.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

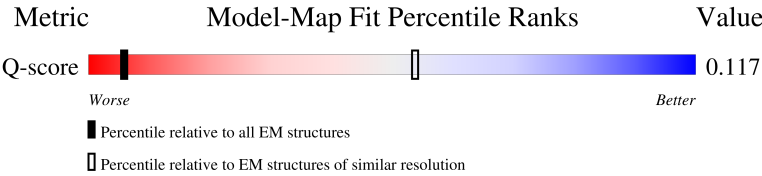
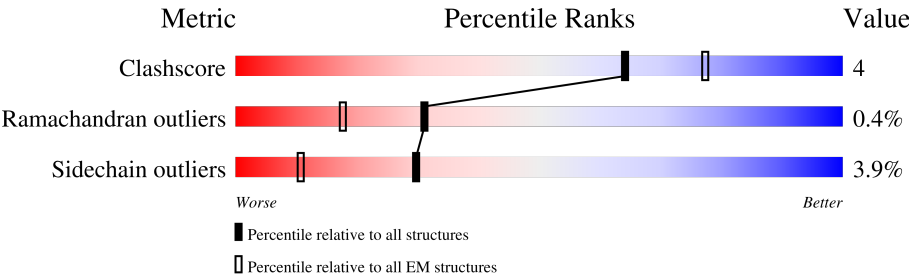
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 8.30 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 280 ( 7.82 - 8.80 )                                      |

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     | 1396   | <div> <div>40%</div> <div>70% 13% 16%</div> </div> |
| 1   | B     | 1396   | <div> <div>45%</div> <div>84% 11% 5%</div> </div>  |
| 1   | D     | 1396   | <div> <div>42%</div> <div>83% 12% . .</div> </div> |
| 1   | F     | 1396   | <div> <div>43%</div> <div>85% 10% . .</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | H     | 1396   |                  |
| 1   | J     | 1396   |                  |
| 1   | L     | 1396   |                  |
| 2   | C     | 235    |                  |
| 2   | E     | 235    |                  |
| 2   | G     | 235    |                  |
| 2   | I     | 235    |                  |
| 2   | K     | 235    |                  |
| 2   | M     | 235    |                  |
| 3   | N     | 483    |                  |
| 3   | Q     | 483    |                  |
| 4   | O     | 316    |                  |
| 4   | P     | 316    |                  |
| 4   | R     | 316    |                  |
| 4   | S     | 316    |                  |
| 5   | T     | 676    |                  |
| 6   | U     | 579    |                  |
| 6   | V     | 579    |                  |
| 7   | W     | 2763   |                  |
| 7   | X     | 2763   |                  |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 102113 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 ORF40.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 1166     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9043  | 5744 | 1576 | 1664 | 59 |         |       |
| 1   | B     | 1332     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10283 | 6529 | 1786 | 1900 | 68 |         |       |
| 1   | D     | 1337     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10245 | 6510 | 1760 | 1909 | 66 |         |       |
| 1   | F     | 1337     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10328 | 6558 | 1786 | 1916 | 68 |         |       |
| 1   | H     | 1281     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9821  | 6246 | 1690 | 1819 | 66 |         |       |
| 1   | J     | 1279     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9850  | 6242 | 1714 | 1829 | 65 |         |       |
| 1   | L     | 1314     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10181 | 6461 | 1766 | 1888 | 66 |         |       |

- Molecule 2 is a protein called Small capsomere-interacting protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | C     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 724   | 461 | 123 | 138 | 2 |         |       |
| 2   | E     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 712   | 452 | 126 | 132 | 2 |         |       |
| 2   | G     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 736   | 467 | 129 | 138 | 2 |         |       |
| 2   | I     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 742   | 470 | 132 | 138 | 2 |         |       |
| 2   | K     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 742   | 470 | 132 | 138 | 2 |         |       |
| 2   | M     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 721   | 459 | 122 | 138 | 2 |         |       |

- Molecule 3 is a protein called ORF20.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | N     | 357      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2767  | 1753 | 483 | 515 | 16 |         |       |
| 3   | Q     | 357      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2770  | 1754 | 484 | 516 | 16 |         |       |

- Molecule 4 is a protein called ORF41.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | O     | 298      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2288  | 1458 | 397 | 422 | 11 |         |       |
| 4   | P     | 275      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2080  | 1333 | 354 | 384 | 9  |         |       |
| 4   | R     | 298      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2288  | 1458 | 397 | 422 | 11 |         |       |
| 4   | S     | 275      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2083  | 1334 | 354 | 386 | 9  |         |       |

- Molecule 5 is a protein called ORF43.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | T     | 593      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4593  | 2943 | 782 | 843 | 25 |         |       |

- Molecule 6 is a protein called ORF34.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | U     | 531      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4200  | 2636 | 745 | 799 | 20 |         |       |
| 6   | V     | 531      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4200  | 2636 | 745 | 799 | 20 |         |       |

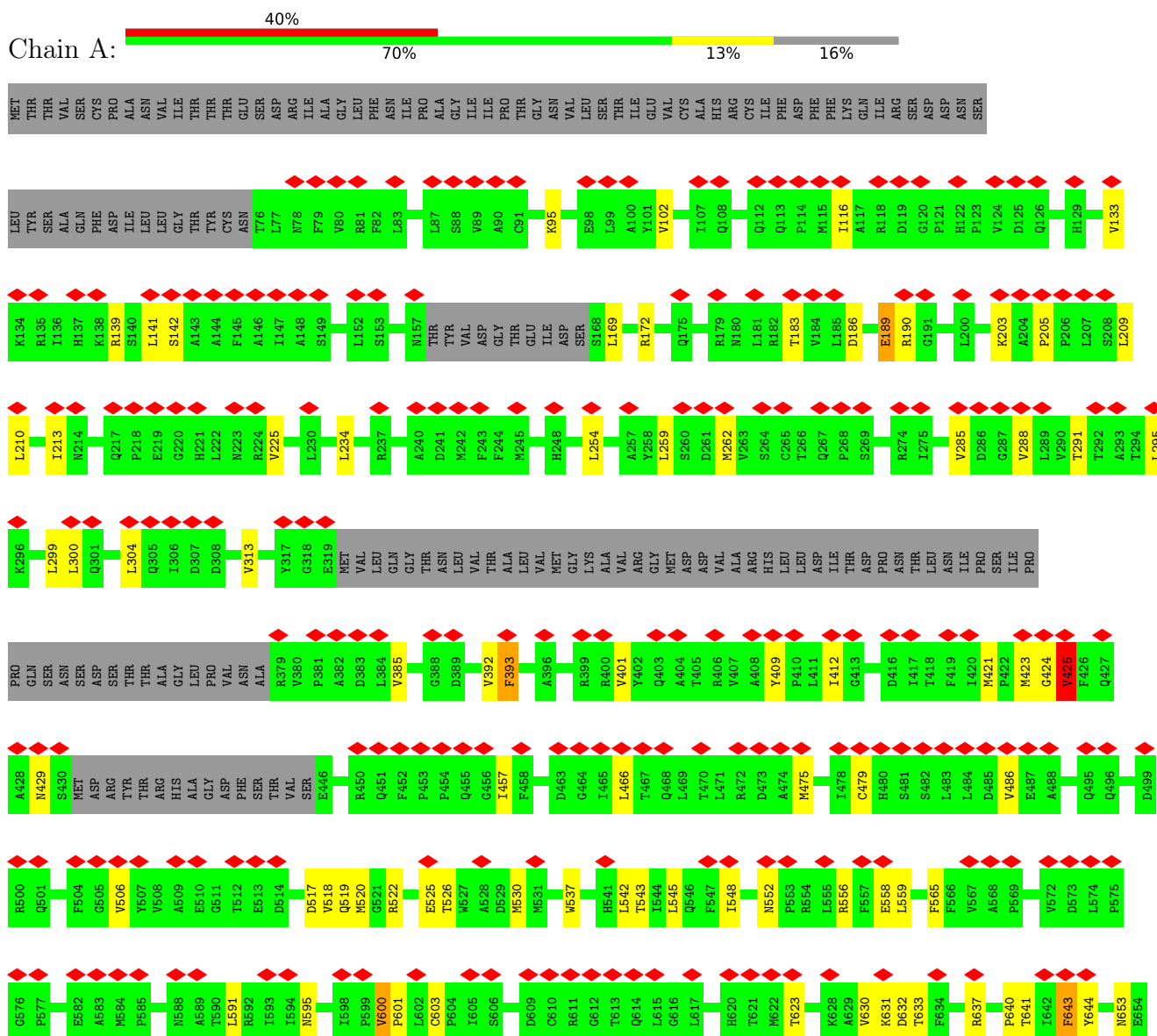
- Molecule 7 is a protein called Large tegument protein deneddylase.

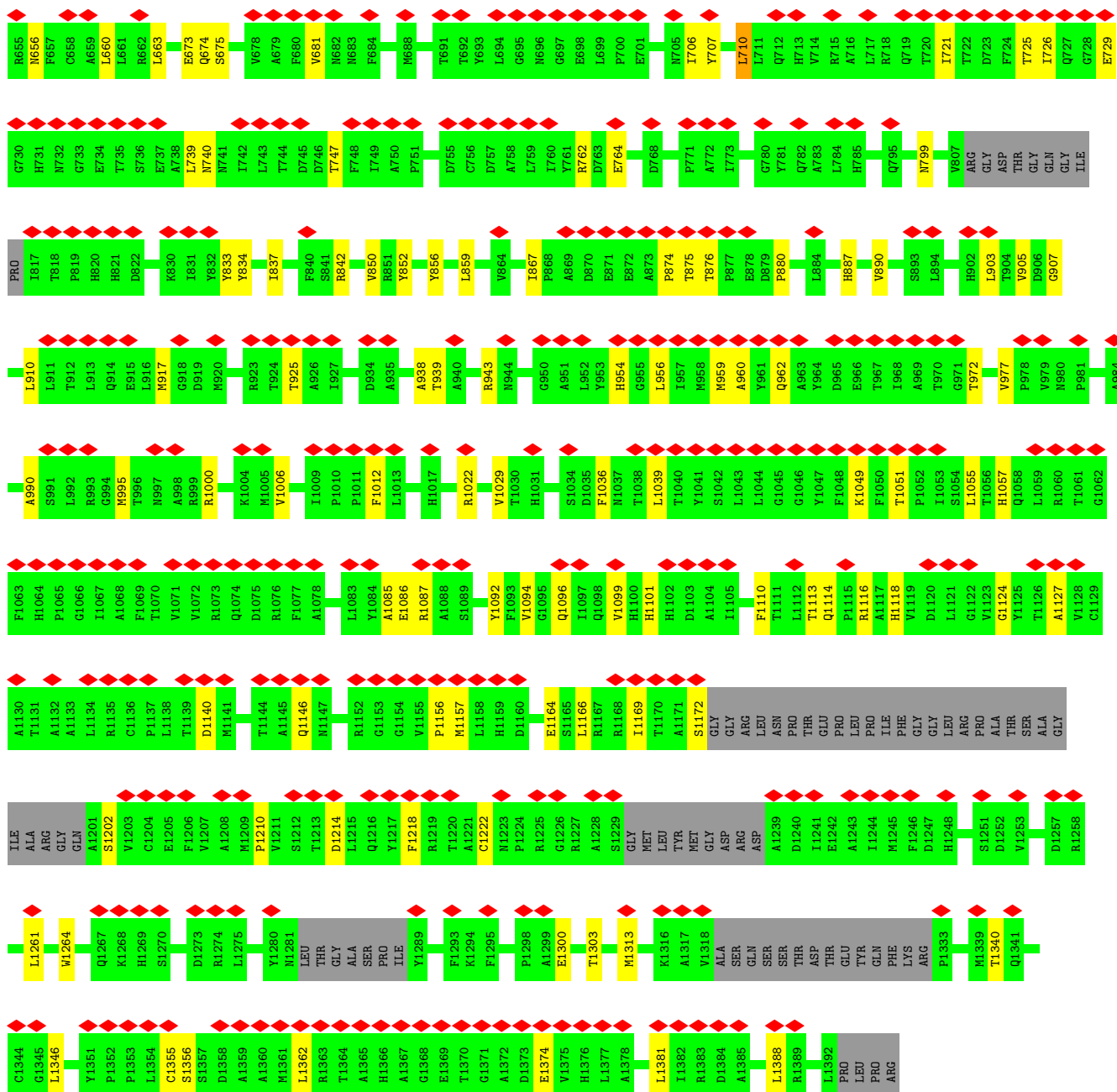
| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | W     | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 358   | 228 | 64 | 63 | 3 |         |       |
| 7   | X     | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 358   | 228 | 64 | 63 | 3 |         |       |

### 3 Residue-property plots

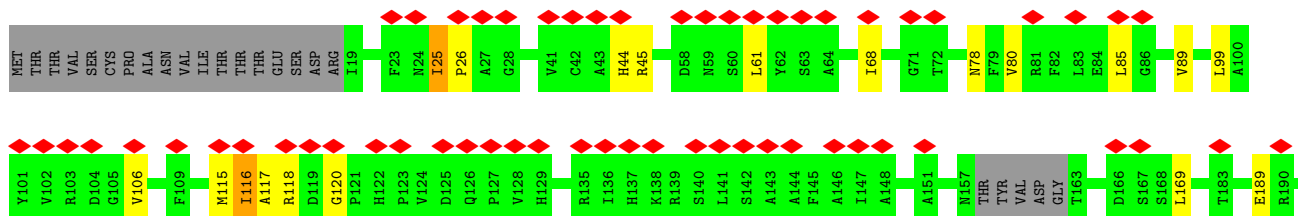
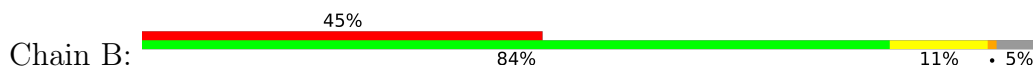
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

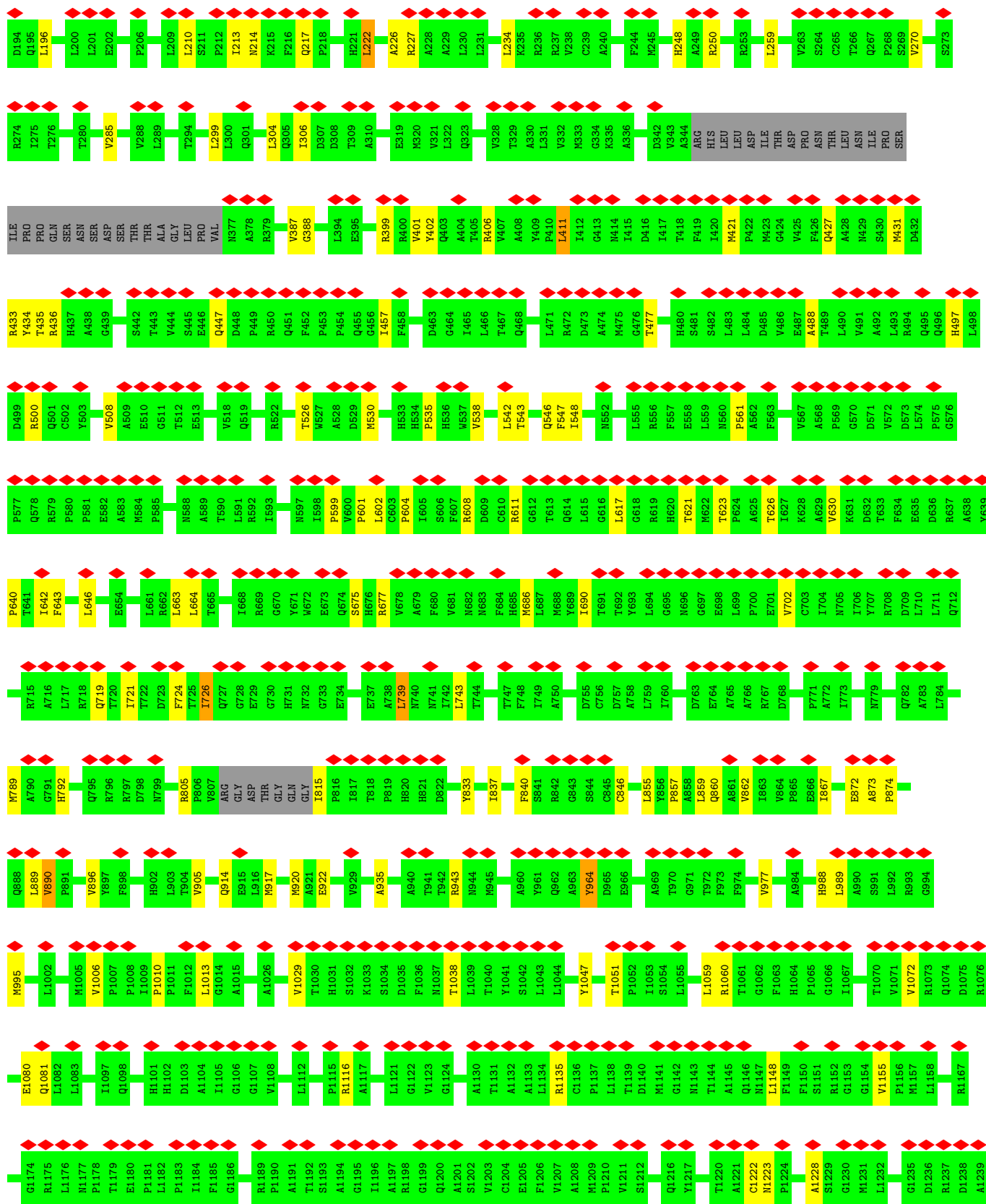
#### • Molecule 1: ORF40

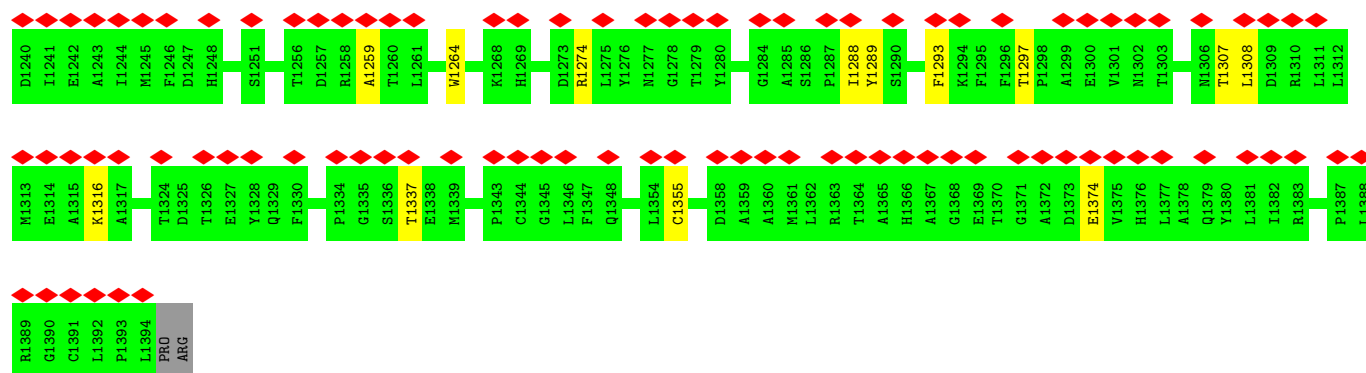




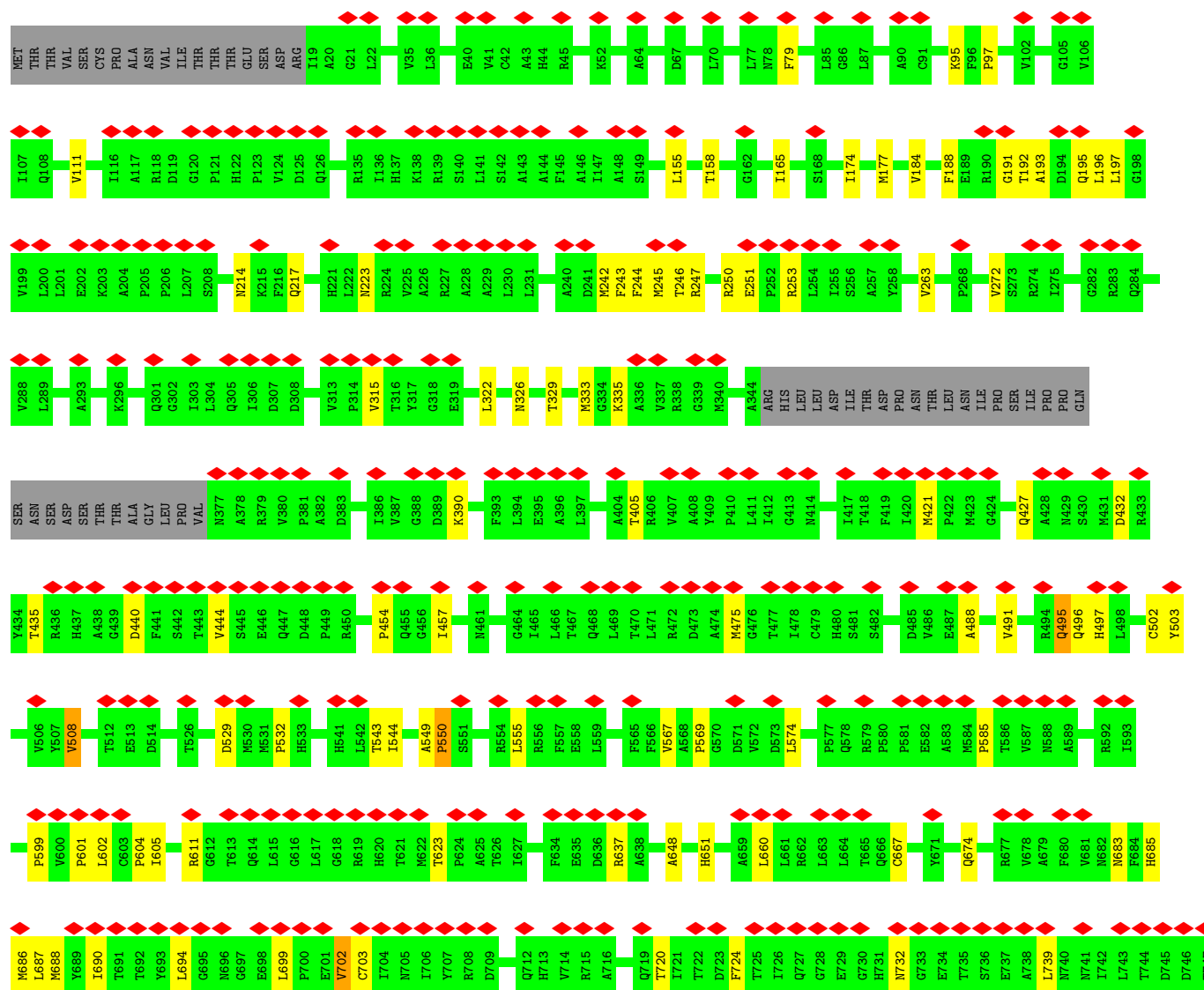
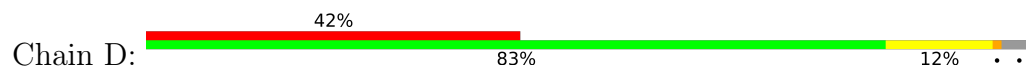
• Molecule 1: ORF40

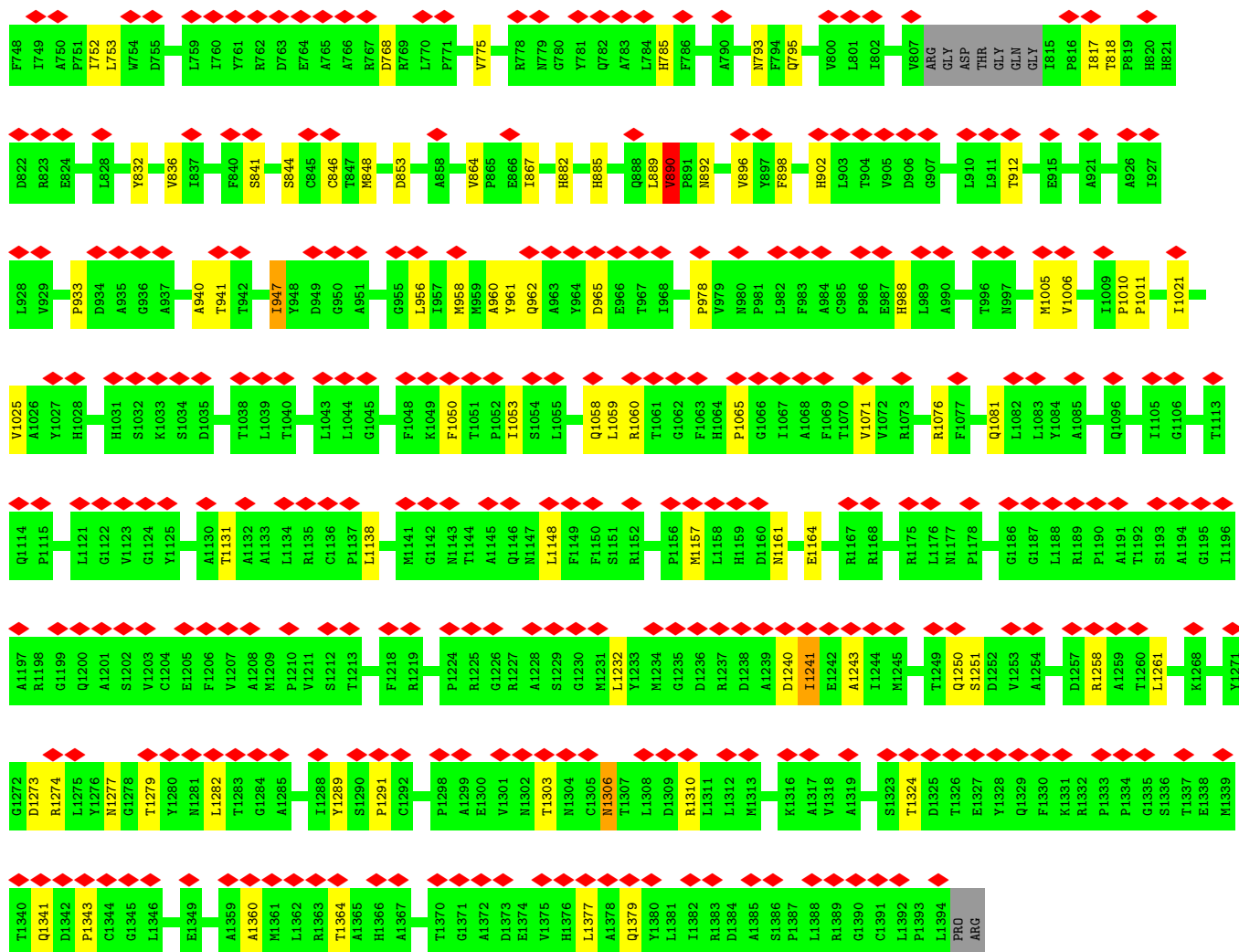




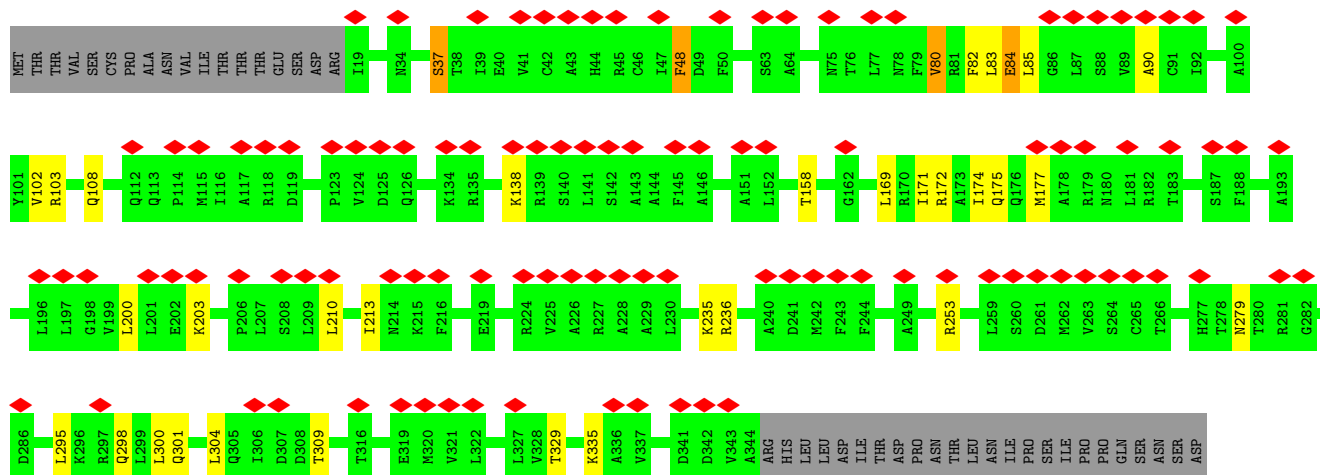
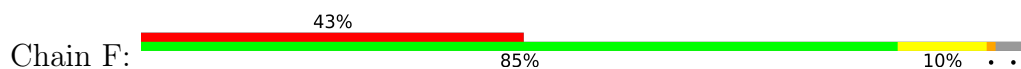


● Molecule 1: ORF40





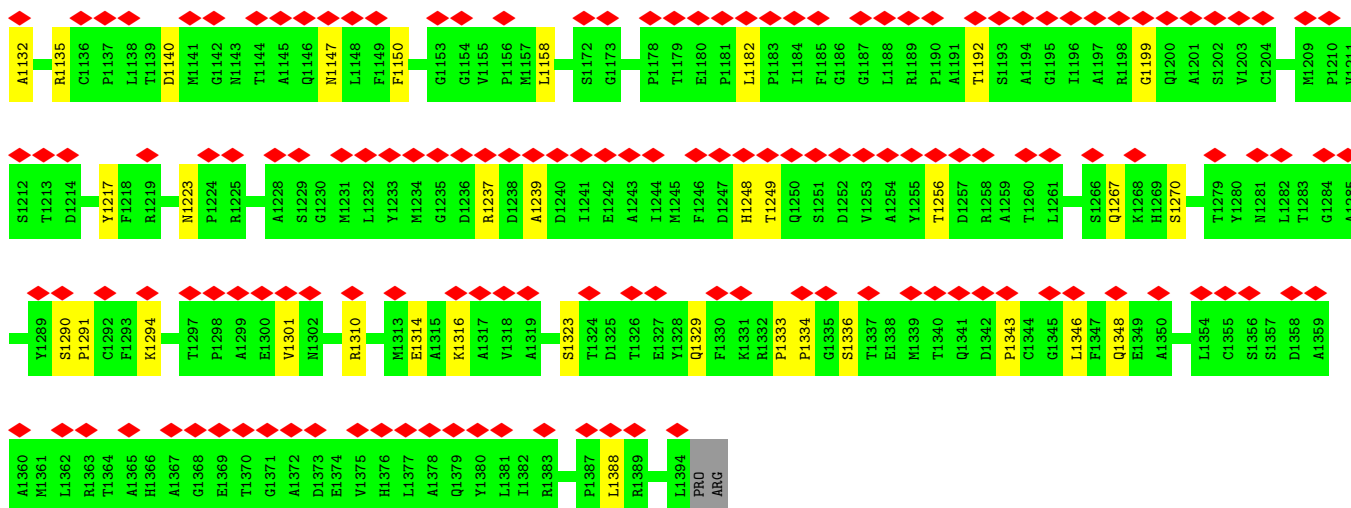
• Molecule 1: ORF40



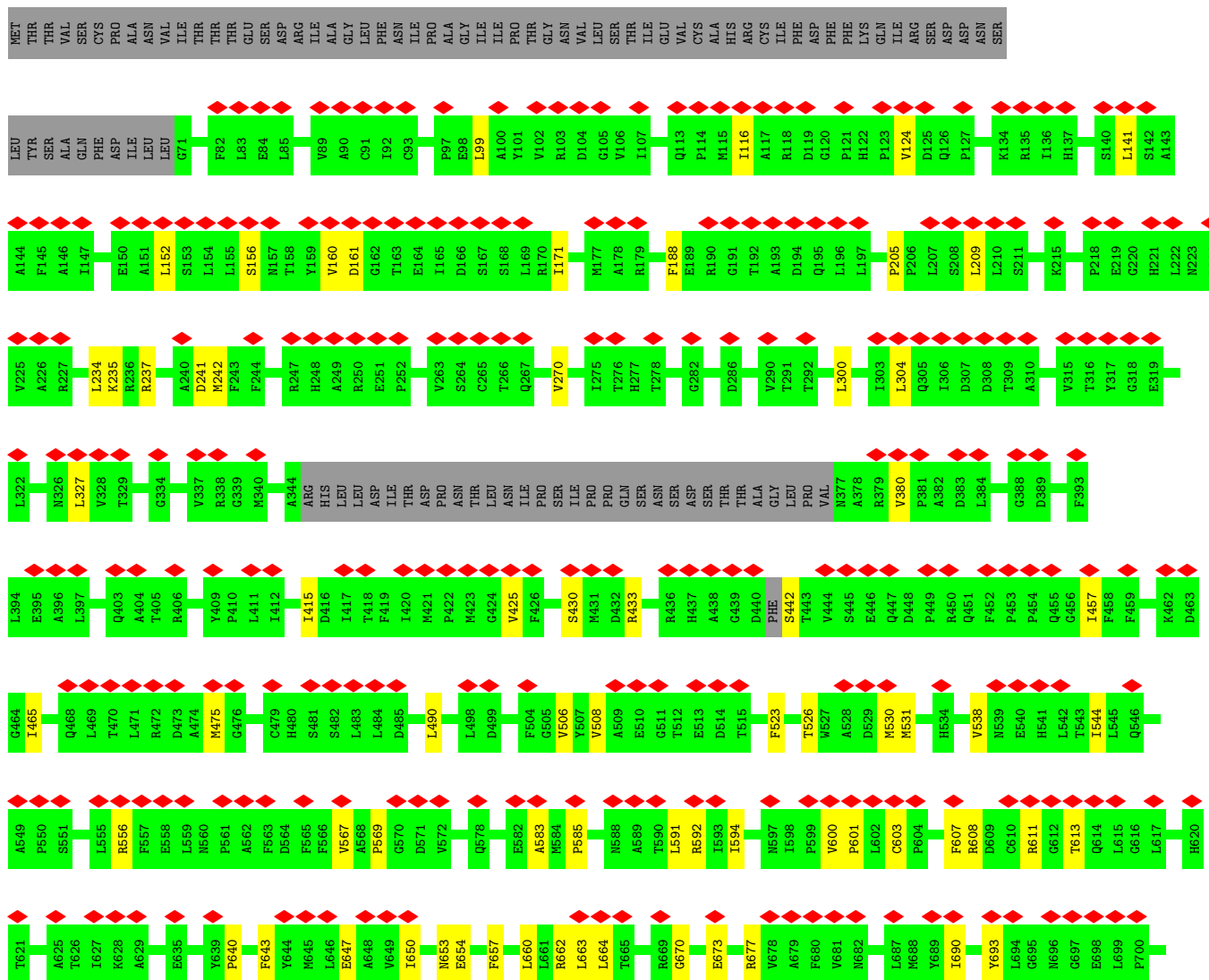
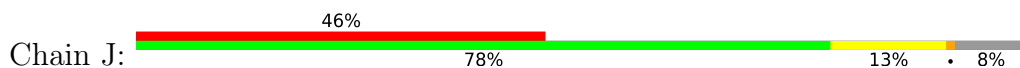


Chain H:

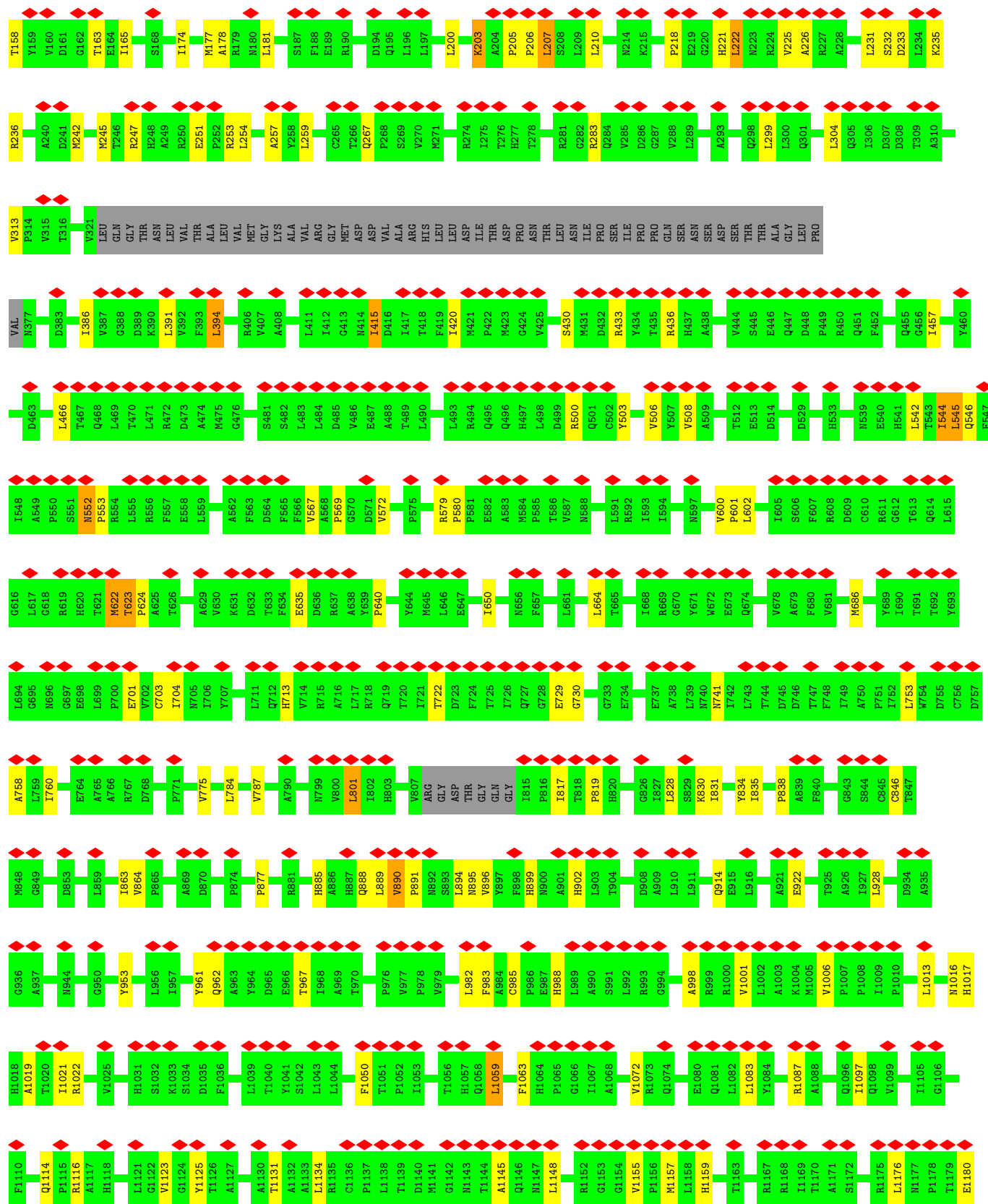




• Molecule 1: ORF40

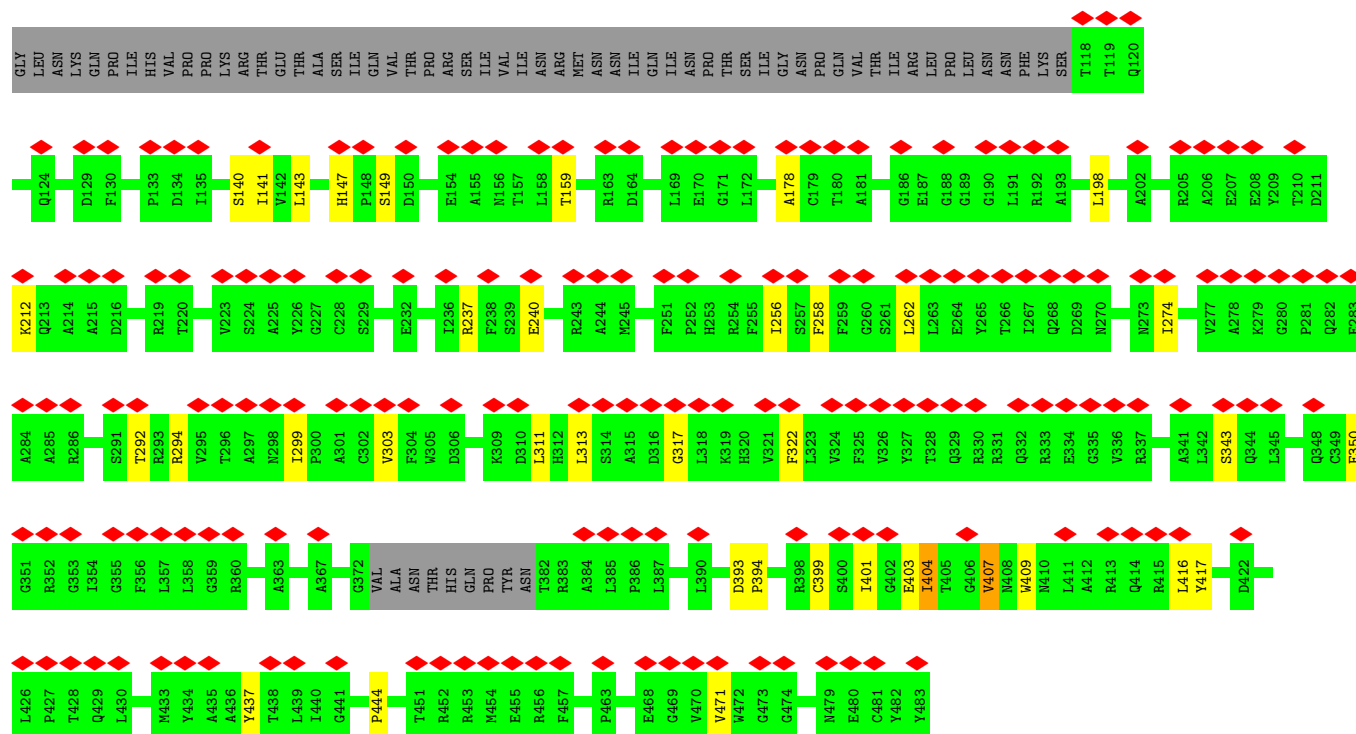




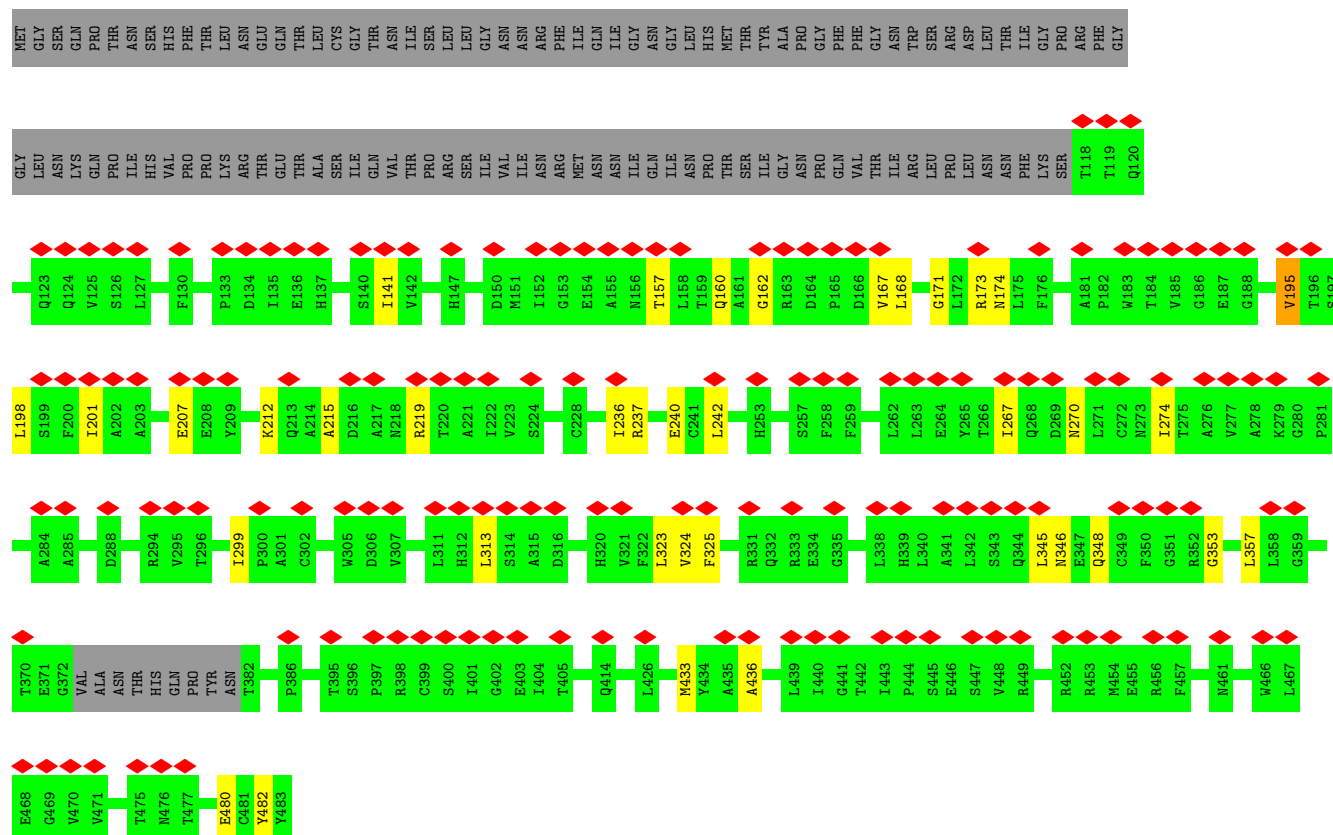




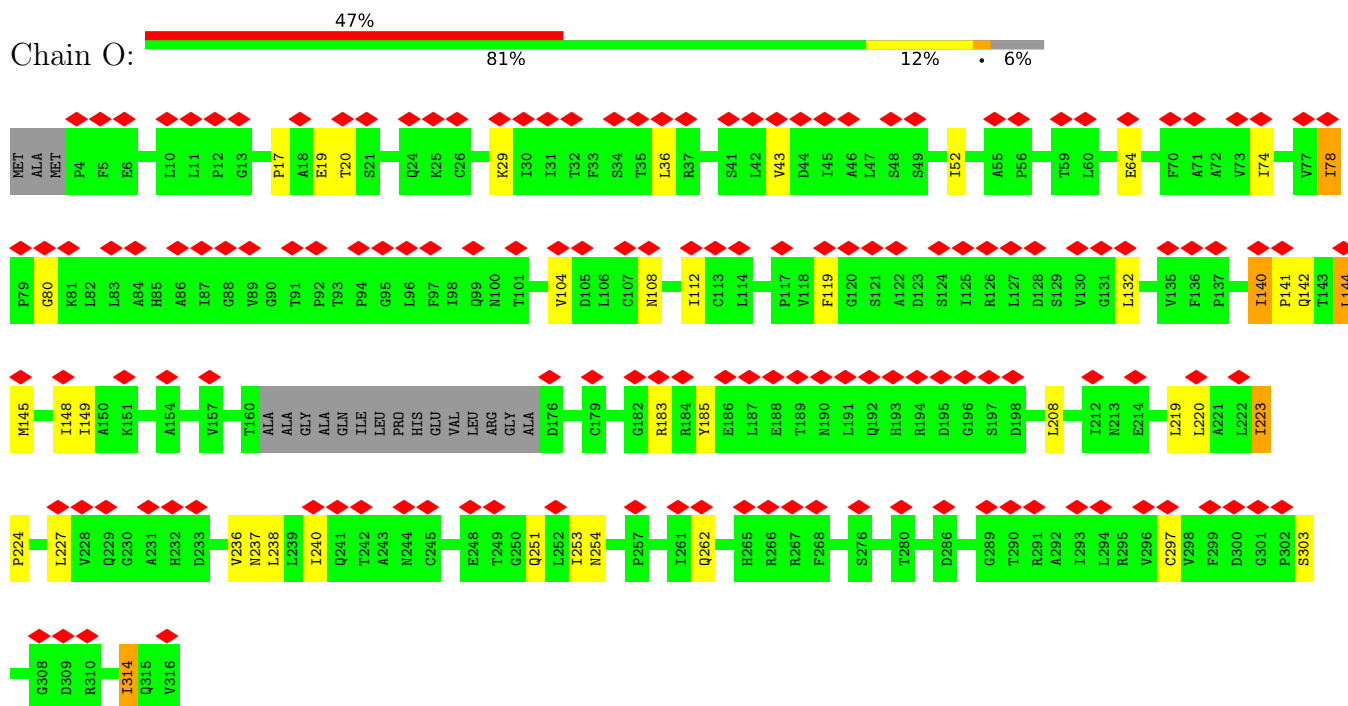
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | GLY | SER | GLN | PRO | THR | ASN | SER | HIS | PHE | THR | LEU | ASN | GLU | GLN | LEU | THR | CYS | GLY | THR | ASN | ASN | ILE | SER | LEU | LEU | GLY | ASN | ASN | ARG | PHE | ILE | ILE | ILE | GLY | ASN | GLY | LEU | HIS | MET | THR | TYR | ALA | PRO | GLY | PHE | PHE | GLY | ASN | TRP | SER | ARG | ASP | LEU | THR | ILE | GLY | PRO | ARG | PHE | TYR |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



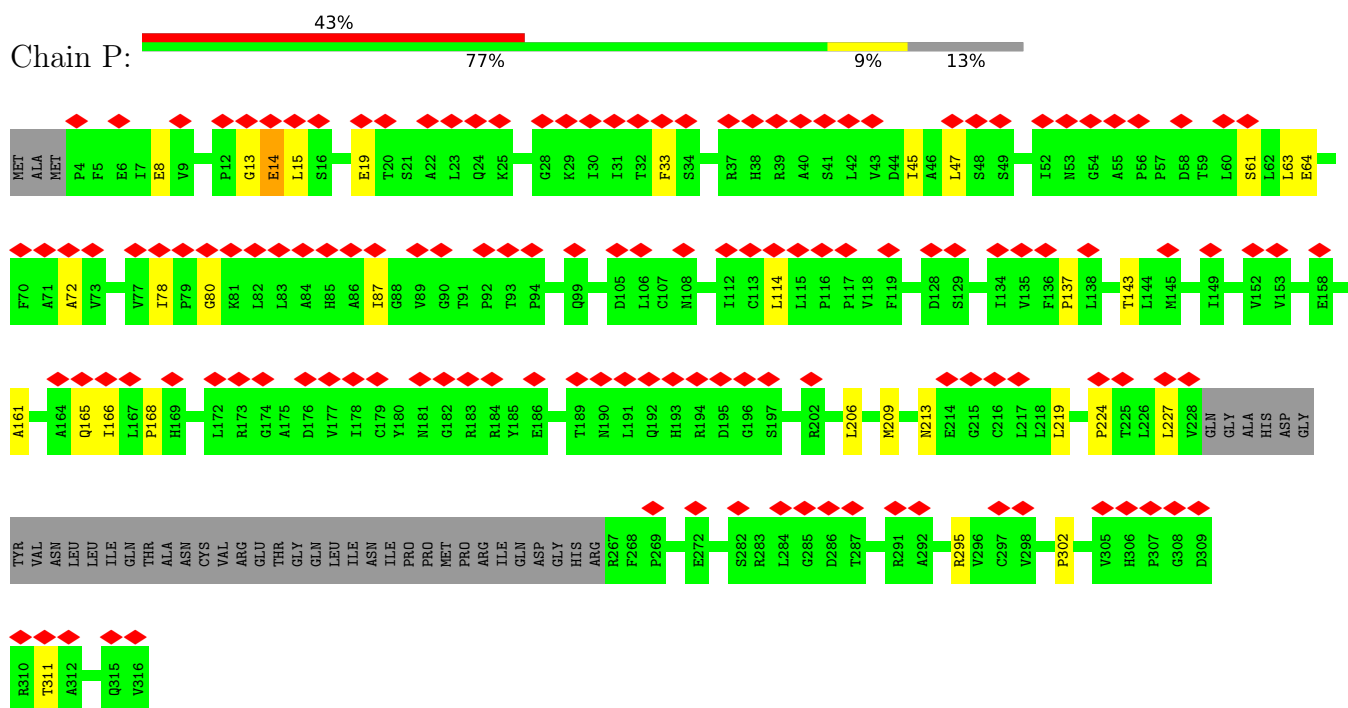
### • Molecule 3: ORF20



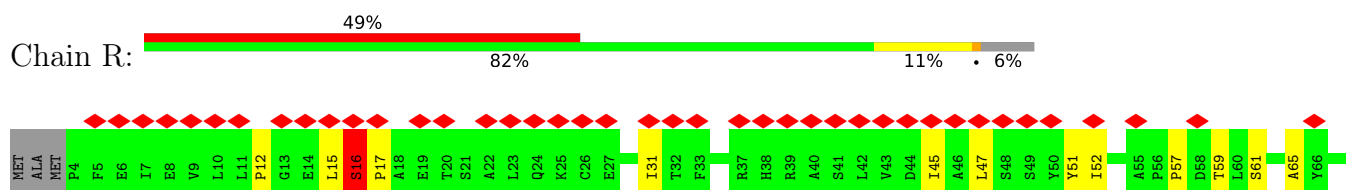
- Molecule 4: ORF41

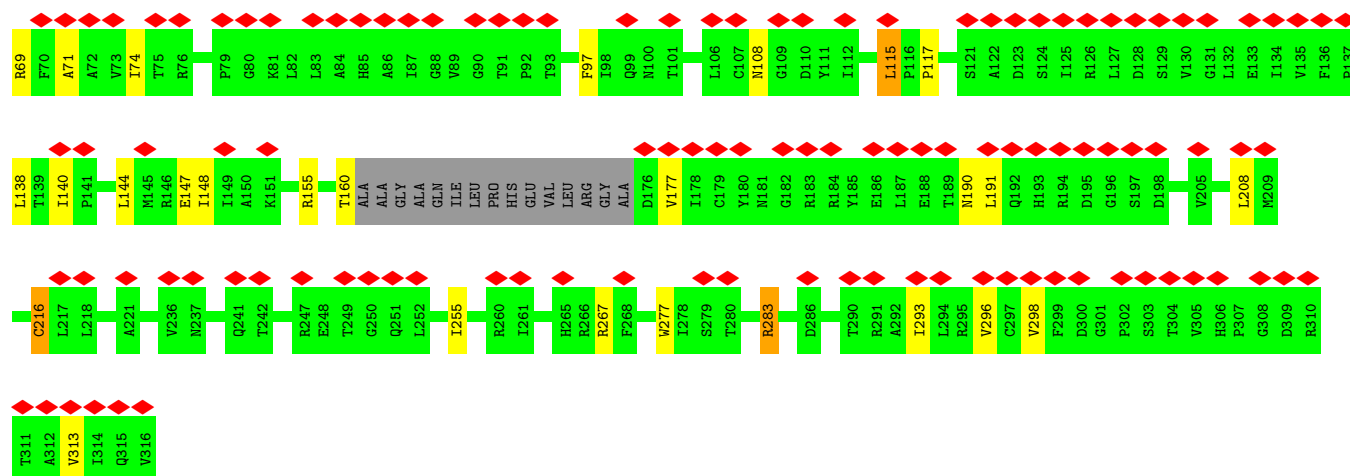


- Molecule 4: ORF41

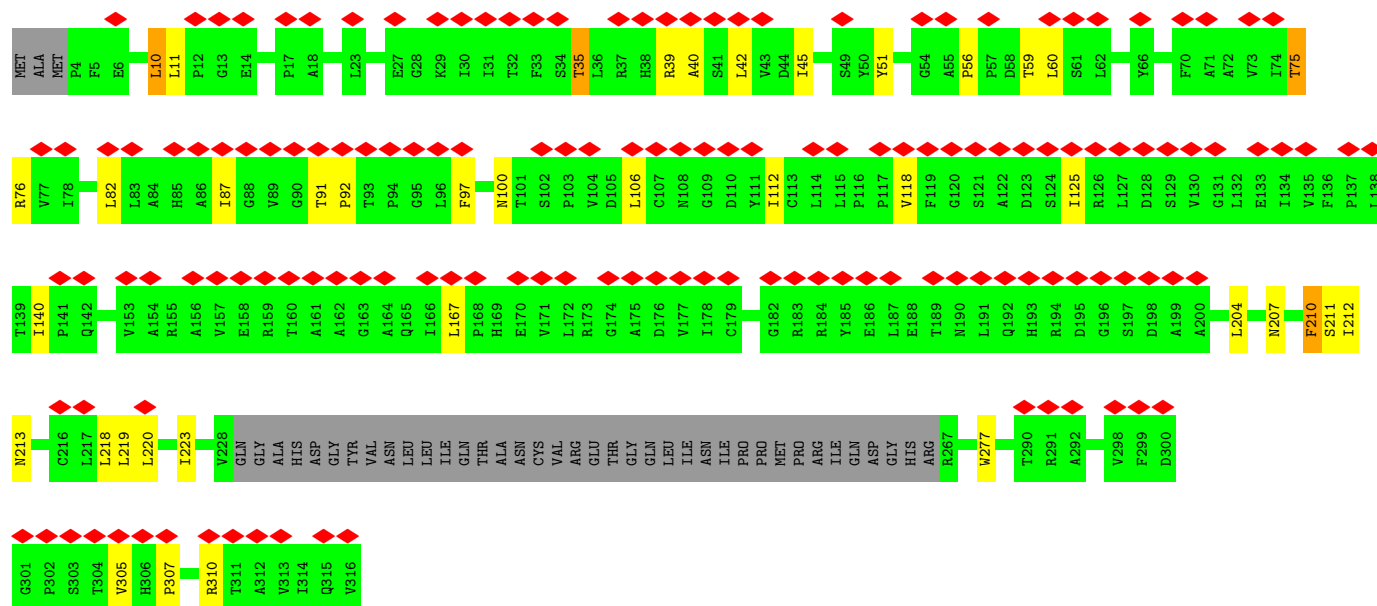
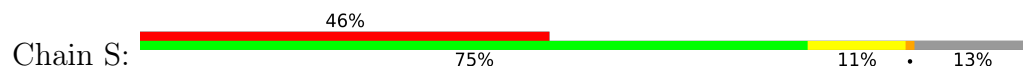


- Molecule 4: ORF41

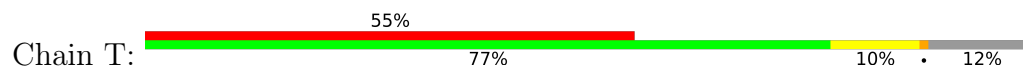


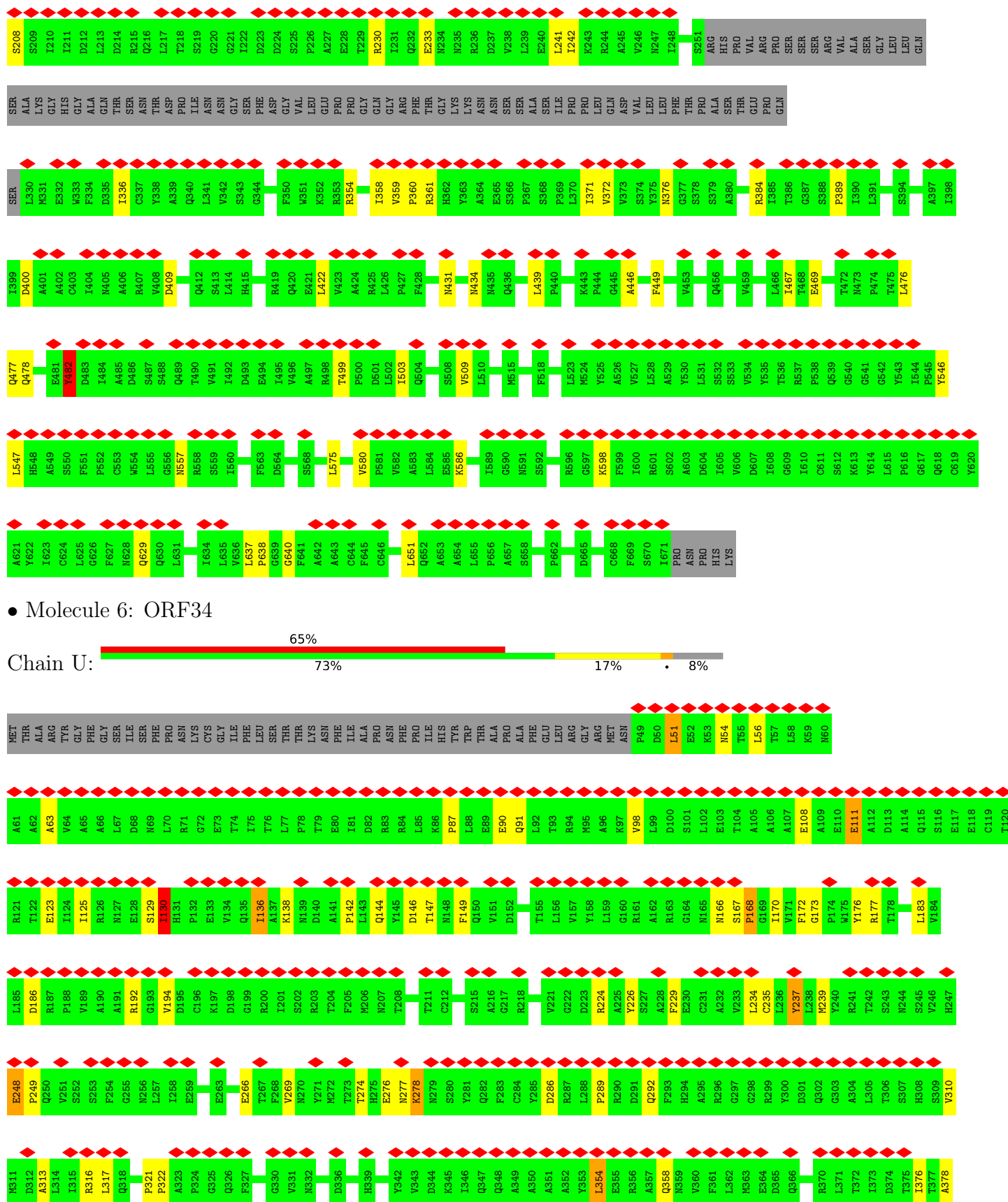


• Molecule 4: ORF41



• Molecule 5: ORF43

















## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SUBTOMOGRAM AVERAGING                   | Depositor |
| Imposed symmetry                     | POINT, C5                               | Depositor |
| Number of subtomograms used          | 3804                                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 82.3                                    | Depositor |
| Minimum defocus (nm)                 | 2000                                    | Depositor |
| Maximum defocus (nm)                 | 5000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 14.690                                  | Depositor |
| Minimum map value                    | -7.382                                  | Depositor |
| Average map value                    | 0.033                                   | Depositor |
| Map value standard deviation         | 0.423                                   | Depositor |
| Recommended contour level            | 1.05                                    | Depositor |
| Map size (Å)                         | 660.48, 660.48, 660.48                  | wwPDB     |
| Map dimensions                       | 192, 192, 192                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 3.4399998, 3.4399998, 3.4399998         | 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     | 0.09         | 0/9259      | 0.23        | 0/12619         |
| 1   | B     | 0.08         | 0/10530     | 0.22        | 0/14358         |
| 1   | D     | 0.15         | 0/10493     | 0.25        | 0/14326         |
| 1   | F     | 0.08         | 0/10575     | 0.21        | 0/14419         |
| 1   | H     | 0.08         | 0/10059     | 0.21        | 0/13730         |
| 1   | J     | 0.09         | 0/10085     | 0.24        | 0/13758         |
| 1   | L     | 0.13         | 0/10430     | 0.26        | 2/14225 (0.0%)  |
| 2   | C     | 0.09         | 0/741       | 0.23        | 0/1022          |
| 2   | E     | 0.10         | 0/727       | 0.25        | 0/997           |
| 2   | G     | 0.09         | 0/753       | 0.22        | 0/1036          |
| 2   | I     | 0.09         | 0/759       | 0.23        | 0/1043          |
| 2   | K     | 0.09         | 0/759       | 0.20        | 0/1043          |
| 2   | M     | 0.10         | 0/738       | 0.25        | 0/1019          |
| 3   | N     | 0.07         | 0/2829      | 0.20        | 0/3850          |
| 3   | Q     | 0.08         | 0/2832      | 0.21        | 0/3854          |
| 4   | O     | 0.08         | 0/2331      | 0.23        | 0/3178          |
| 4   | P     | 0.09         | 0/2119      | 0.21        | 0/2892          |
| 4   | R     | 0.08         | 0/2331      | 0.22        | 0/3178          |
| 4   | S     | 0.08         | 0/2122      | 0.22        | 0/2896          |
| 5   | T     | 0.08         | 0/4700      | 0.23        | 0/6406          |
| 6   | U     | 0.11         | 0/4277      | 0.30        | 0/5806          |
| 6   | V     | 0.15         | 0/4277      | 0.32        | 0/5806          |
| 7   | W     | 0.06         | 0/361       | 0.12        | 0/484           |
| 7   | X     | 0.07         | 0/361       | 0.15        | 0/484           |
| All | All   | 0.10         | 0/104448    | 0.24        | 2/142429 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | L     | 1377 | LEU  | CA-C-N | -5.41 | 115.13      | 123.14   |
| 1   | L     | 1377 | LEU  | C-N-CA | -5.41 | 115.13      | 123.14   |

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     | 9043   | 0        | 8818     | 81      | 0            |
| 1   | B     | 10283  | 0        | 10047    | 73      | 0            |
| 1   | D     | 10245  | 0        | 9938     | 83      | 0            |
| 1   | F     | 10328  | 0        | 10090    | 71      | 0            |
| 1   | H     | 9821   | 0        | 9535     | 71      | 0            |
| 1   | J     | 9850   | 0        | 9593     | 101     | 0            |
| 1   | L     | 10181  | 0        | 9923     | 103     | 0            |
| 2   | C     | 724    | 0        | 696      | 2       | 0            |
| 2   | E     | 712    | 0        | 706      | 7       | 0            |
| 2   | G     | 736    | 0        | 718      | 5       | 0            |
| 2   | I     | 742    | 0        | 729      | 4       | 0            |
| 2   | K     | 742    | 0        | 729      | 10      | 0            |
| 2   | M     | 721    | 0        | 687      | 4       | 0            |
| 3   | N     | 2767   | 0        | 2675     | 22      | 0            |
| 3   | Q     | 2770   | 0        | 2679     | 21      | 0            |
| 4   | O     | 2288   | 0        | 2352     | 25      | 0            |
| 4   | P     | 2080   | 0        | 2136     | 16      | 0            |
| 4   | R     | 2288   | 0        | 2352     | 21      | 0            |
| 4   | S     | 2083   | 0        | 2138     | 18      | 0            |
| 5   | T     | 4593   | 0        | 4609     | 39      | 0            |
| 6   | U     | 4200   | 0        | 4166     | 64      | 0            |
| 6   | V     | 4200   | 0        | 4166     | 61      | 0            |
| 7   | W     | 358    | 0        | 379      | 3       | 0            |
| 7   | X     | 358    | 0        | 379      | 9       | 0            |
| All | All   | 102113 | 0        | 100240   | 834     | 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 4.

All (834) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:J:898:PHE:O     | 1:J:902:HIS:HB3  | 1.66                     | 0.96              |
| 1:J:737:GLU:O     | 1:J:741:ASN:HB2  | 1.69                     | 0.93              |
| 1:B:25:ILE:HG13   | 1:B:26:PRO:HD3   | 1.59                     | 0.85              |
| 1:D:602:LEU:HG    | 1:D:605:ILE:HD12 | 1.64                     | 0.80              |
| 6:U:248:GLU:H     | 6:U:249:PRO:HD2  | 1.50                     | 0.77              |
| 1:F:1243:ALA:O    | 1:F:1247:ASP:HB2 | 1.85                     | 0.76              |
| 3:Q:353:GLY:O     | 3:Q:357:LEU:HB2  | 1.88                     | 0.74              |
| 1:J:1006:VAL:HG23 | 1:J:1007:PRO:HD3 | 1.69                     | 0.73              |
| 6:V:439:LEU:O     | 6:V:443:TYR:HB2  | 1.90                     | 0.71              |
| 1:B:120:GLY:HA2   | 1:D:195:GLN:HB2  | 1.73                     | 0.70              |
| 1:A:291:THR:HG21  | 1:A:295:LEU:HB2  | 1.74                     | 0.69              |
| 1:H:1310:ARG:O    | 1:H:1314:GLU:HB2 | 1.92                     | 0.69              |
| 1:J:640:PRO:HB2   | 1:J:643:PHE:HB2  | 1.74                     | 0.69              |
| 1:B:543:THR:HA    | 1:B:546:GLN:HG2  | 1.76                     | 0.68              |
| 6:V:389:GLY:HA3   | 6:V:435:ASN:HD22 | 1.58                     | 0.68              |
| 5:T:557:ASN:H     | 5:T:629:GLN:HB3  | 1.58                     | 0.68              |
| 1:A:299:LEU:HD12  | 1:A:304:LEU:HG   | 1.75                     | 0.68              |
| 1:J:526:THR:O     | 1:J:530:MET:HB2  | 1.93                     | 0.67              |
| 1:L:1123:VAL:HG13 | 1:L:1125:TYR:H   | 1.59                     | 0.67              |
| 1:D:599:PRO:HB2   | 1:D:604:PRO:HD3  | 1.77                     | 0.66              |
| 5:T:207:VAL:HG13  | 5:T:208:SER:H    | 1.61                     | 0.66              |
| 3:N:292:THR:HG23  | 3:N:294:ARG:H    | 1.61                     | 0.65              |
| 1:D:1241:ILE:HG23 | 1:D:1243:ALA:H   | 1.62                     | 0.65              |
| 1:L:760:ILE:HG21  | 1:L:819:PRO:HG3  | 1.79                     | 0.65              |
| 3:Q:160:GLN:HG2   | 3:Q:162:GLY:H    | 1.61                     | 0.65              |
| 1:J:747:THR:HG21  | 1:J:931:SER:HB3  | 1.79                     | 0.64              |
| 4:P:161:ALA:O     | 4:P:165:GLN:HB2  | 1.96                     | 0.64              |
| 4:O:237:ASN:HA    | 4:O:240:ILE:HG12 | 1.80                     | 0.64              |
| 1:J:237:ARG:O     | 1:J:241:ASP:HB3  | 1.98                     | 0.63              |
| 6:V:495:LEU:HD12  | 6:V:525:VAL:HG22 | 1.80                     | 0.63              |
| 5:T:41:LEU:HD23   | 5:T:45:LYS:HB3   | 1.80                     | 0.63              |
| 1:J:712:GLN:HG3   | 1:L:635:GLU:HG2  | 1.81                     | 0.63              |
| 2:K:96:VAL:HB     | 1:L:895:ASN:HB2  | 1.79                     | 0.62              |
| 6:U:144:GLN:HE21  | 6:U:149:PHE:H    | 1.47                     | 0.62              |
| 1:H:868:PRO:HB2   | 1:H:871:GLU:HB2  | 1.80                     | 0.62              |
| 1:F:817:ILE:HG12  | 1:F:819:PRO:HD2  | 1.81                     | 0.62              |
| 1:J:300:LEU:HA    | 1:J:304:LEU:HB2  | 1.80                     | 0.62              |
| 1:J:710:LEU:HA    | 1:J:713:HIS:HD2  | 1.65                     | 0.62              |
| 1:H:420:ILE:HG23  | 1:H:422:PRO:HD3  | 1.82                     | 0.62              |
| 1:D:193:ALA:HA    | 1:D:196:LEU:HB3  | 1.81                     | 0.62              |
| 6:U:183:LEU:HA    | 6:U:186:ASP:HB2  | 1.81                     | 0.62              |
| 1:L:579:ARG:HH11  | 1:L:580:PRO:HD2  | 1.65                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:663:LEU:HD12 | 1:J:909:ALA:HB1   | 1.81                     | 0.61              |
| 1:D:611:ARG:HH12 | 1:D:1065:PRO:HA   | 1.63                     | 0.61              |
| 6:U:413:PRO:HB3  | 6:U:417:VAL:HB    | 1.81                     | 0.61              |
| 6:V:340:THR:HB   | 6:V:368:LEU:HB3   | 1.82                     | 0.61              |
| 1:A:660:LEU:HD23 | 1:A:663:LEU:HD21  | 1.82                     | 0.61              |
| 1:L:552:ASN:H    | 1:L:553:PRO:HD2   | 1.66                     | 0.61              |
| 6:V:143:LEU:HB3  | 6:V:406:VAL:HG22  | 1.82                     | 0.61              |
| 1:D:694:LEU:HD21 | 1:D:699:LEU:HD23  | 1.83                     | 0.61              |
| 1:F:1142:GLY:HA3 | 1:F:1202:SER:H    | 1.66                     | 0.61              |
| 1:A:139:ARG:HH22 | 1:A:141:LEU:HD12  | 1.66                     | 0.60              |
| 1:B:526:THR:O    | 1:B:530:MET:HB2   | 2.01                     | 0.60              |
| 1:D:898:PHE:O    | 1:D:902:HIS:HB3   | 2.01                     | 0.60              |
| 6:U:277:ASN:HB2  | 6:U:386:LEU:HB2   | 1.83                     | 0.60              |
| 3:N:299:ILE:HB   | 3:N:303:VAL:HG11  | 1.81                     | 0.60              |
| 1:F:1104:ALA:HB2 | 1:F:1109:ASN:HB2  | 1.83                     | 0.60              |
| 1:D:785:HIS:HD2  | 1:D:817:ILE:HG13  | 1.66                     | 0.60              |
| 1:F:429:ASN:HD21 | 1:F:432:ASP:HB3   | 1.67                     | 0.60              |
| 1:L:885:HIS:HA   | 1:L:888:GLN:HG3   | 1.83                     | 0.60              |
| 1:D:846:CYS:HB2  | 1:D:988:HIS:HD2   | 1.66                     | 0.60              |
| 4:R:31:ILE:HG12  | 4:R:74:ILE:HD11   | 1.84                     | 0.59              |
| 1:H:1084:TYR:HB3 | 1:H:1128:VAL:HG23 | 1.83                     | 0.59              |
| 6:U:125:ILE:HG23 | 6:U:224:ARG:HD3   | 1.85                     | 0.59              |
| 1:H:415:ILE:HG22 | 1:H:1343:PRO:HG3  | 1.83                     | 0.59              |
| 1:D:933:PRO:HG3  | 1:D:947:ILE:HG12  | 1.85                     | 0.59              |
| 1:J:1086:GLU:HB2 | 1:J:1089:SER:HB2  | 1.84                     | 0.59              |
| 6:U:172:PHE:HB2  | 6:U:176:TYR:HB2   | 1.84                     | 0.59              |
| 1:L:760:ILE:HD11 | 1:L:817:ILE:HG23  | 1.85                     | 0.59              |
| 1:L:1224:PRO:HG3 | 1:L:1348:GLN:HB3  | 1.85                     | 0.59              |
| 1:J:205:PRO:HG2  | 1:J:1129:CYS:H    | 1.67                     | 0.58              |
| 1:J:976:PRO:HD2  | 1:J:992:LEU:HD13  | 1.85                     | 0.58              |
| 2:K:99:LYS:HE3   | 1:L:891:PRO:HB3   | 1.85                     | 0.58              |
| 2:I:98:LEU:HD13  | 1:J:896:VAL:HG12  | 1.85                     | 0.58              |
| 1:J:415:ILE:HG22 | 1:J:1077:PHE:H    | 1.68                     | 0.58              |
| 3:Q:215:ALA:HB1  | 3:Q:219:ARG:HH21  | 1.67                     | 0.58              |
| 6:V:332:ASN:HA   | 6:V:336:ASP:HB2   | 1.85                     | 0.58              |
| 1:D:739:LEU:HD22 | 1:D:1050:PHE:HB2  | 1.86                     | 0.58              |
| 1:L:299:LEU:HD13 | 1:L:394:LEU:HD11  | 1.86                     | 0.58              |
| 1:H:471:LEU:HD21 | 1:H:1059:LEU:HB3  | 1.86                     | 0.58              |
| 1:J:611:ARG:HH12 | 1:J:1042:SER:HA   | 1.69                     | 0.58              |
| 4:O:220:LEU:HD13 | 4:O:253:ILE:HG12  | 1.86                     | 0.58              |
| 1:A:423:MET:HE2  | 1:A:457:ILE:HG21  | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:600:VAL:HG13  | 1:A:601:PRO:HD3   | 1.86                     | 0.58              |
| 6:U:173:GLY:HA2   | 6:U:573:PRO:HA    | 1.85                     | 0.58              |
| 1:A:558:GLU:HA    | 1:A:565:PHE:HB2   | 1.86                     | 0.58              |
| 1:B:640:PRO:HD2   | 1:B:643:PHE:HB2   | 1.85                     | 0.58              |
| 1:J:1267:GLN:HE22 | 1:J:1270:SER:HB2  | 1.68                     | 0.57              |
| 4:O:208:LEU:HB3   | 4:P:219:LEU:HD12  | 1.85                     | 0.57              |
| 6:U:183:LEU:HD22  | 6:U:192:ARG:HB2   | 1.86                     | 0.57              |
| 3:Q:207:GLU:HA    | 3:Q:212:LYS:HD3   | 1.86                     | 0.57              |
| 1:D:882:HIS:HB3   | 1:D:885:HIS:HB2   | 1.87                     | 0.57              |
| 4:S:35:THR:HB     | 4:S:40:ALA:HB2    | 1.85                     | 0.57              |
| 1:D:1341:GLN:HG3  | 1:D:1343:PRO:HD3  | 1.86                     | 0.57              |
| 1:J:99:LEU:HD13   | 1:J:1095:GLY:HA3  | 1.87                     | 0.57              |
| 1:H:213:ILE:HD11  | 1:H:237:ARG:HG3   | 1.87                     | 0.57              |
| 1:L:415:ILE:HG23  | 1:L:1343:PRO:HG3  | 1.87                     | 0.57              |
| 1:B:115:MET:HG2   | 1:D:184:VAL:HG13  | 1.87                     | 0.56              |
| 1:J:1152:ARG:HH12 | 1:J:1184:ILE:HD13 | 1.70                     | 0.56              |
| 1:A:1374:GLU:HA   | 1:A:1381:LEU:HB2  | 1.86                     | 0.56              |
| 1:B:601:PRO:HA    | 1:B:604:PRO:HG3   | 1.88                     | 0.56              |
| 1:D:253:ARG:HH12  | 1:F:298:GLN:HG2   | 1.71                     | 0.56              |
| 1:D:637:ARG:HA    | 1:D:960:ALA:HB1   | 1.86                     | 0.56              |
| 1:J:1121:LEU:HD13 | 1:J:1123:VAL:HG12 | 1.87                     | 0.56              |
| 1:J:734:GLU:HG2   | 1:J:738:ALA:H     | 1.71                     | 0.56              |
| 4:R:115:LEU:HD21  | 4:R:140:ILE:HB    | 1.88                     | 0.56              |
| 3:Q:433:MET:HA    | 3:Q:482:TYR:HB3   | 1.87                     | 0.56              |
| 6:U:183:LEU:HB3   | 6:U:192:ARG:HD3   | 1.86                     | 0.56              |
| 1:B:889:LEU:HD23  | 2:E:98:LEU:HB2    | 1.87                     | 0.56              |
| 1:A:537:TRP:CD1   | 1:A:1022:ARG:HH21 | 2.23                     | 0.56              |
| 1:J:1010:PRO:HG2  | 1:J:1013:LEU:HB2  | 1.88                     | 0.56              |
| 4:R:65:ALA:HB1    | 4:R:69:ARG:HE     | 1.71                     | 0.56              |
| 4:R:57:PRO:HG2    | 4:R:61:SER:HB3    | 1.87                     | 0.56              |
| 6:U:98:VAL:HG11   | 7:X:7:LEU:HD22    | 1.87                     | 0.56              |
| 1:B:431:MET:HB3   | 1:D:1360:ALA:HB2  | 1.88                     | 0.55              |
| 1:D:1050:PHE:HB3  | 1:D:1053:ILE:HG22 | 1.88                     | 0.55              |
| 1:D:1306:ASN:O    | 1:D:1310:ARG:HB2  | 2.05                     | 0.55              |
| 4:O:145:MET:HA    | 4:O:148:ILE:HG12  | 1.87                     | 0.55              |
| 1:D:720:THR:O     | 1:D:724:PHE:HB2   | 2.05                     | 0.55              |
| 1:J:664:LEU:HD23  | 1:J:690:ILE:HD11  | 1.88                     | 0.55              |
| 6:V:208:THR:HA    | 6:V:212:CYS:HB2   | 1.87                     | 0.55              |
| 1:J:1180:GLU:H    | 1:J:1181:PRO:HD2  | 1.70                     | 0.55              |
| 1:L:163:THR:HG23  | 1:L:165:ILE:H     | 1.71                     | 0.55              |
| 3:Q:157:THR:HG23  | 4:R:267:ARG:HB2   | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:V:494:ARG:HB3   | 6:V:521:ILE:HG23  | 1.88                     | 0.55              |
| 5:T:409:ASP:HB2   | 7:W:42:LEU:HD13   | 1.88                     | 0.55              |
| 1:H:560:ASN:H     | 1:H:565:PHE:HZ    | 1.54                     | 0.55              |
| 4:R:59:THR:HG21   | 4:R:190:ASN:HD21  | 1.71                     | 0.55              |
| 1:B:427:GLN:HE21  | 1:B:433:ARG:HE    | 1.55                     | 0.55              |
| 1:B:210:LEU:HA    | 1:B:213:ILE:HG22  | 1.89                     | 0.55              |
| 1:J:670:GLY:HA3   | 1:J:903:LEU:HD21  | 1.89                     | 0.55              |
| 1:L:623:THR:HG23  | 1:L:624:PRO:HD3   | 1.88                     | 0.55              |
| 1:H:1267:GLN:HB2  | 1:H:1270:SER:HB3  | 1.89                     | 0.54              |
| 6:V:504:GLU:HG3   | 6:V:513:LEU:HD12  | 1.89                     | 0.54              |
| 1:A:518:VAL:HG21  | 6:U:521:ILE:HG22  | 1.89                     | 0.54              |
| 1:D:848:MET:HE3   | 1:D:988:HIS:HB3   | 1.87                     | 0.54              |
| 6:V:103:GLU:HG3   | 7:X:5:LEU:HD13    | 1.88                     | 0.54              |
| 1:J:662:ARG:HB2   | 2:K:101:THR:HG23  | 1.88                     | 0.54              |
| 1:J:860:GLN:HE22  | 2:K:62:ALA:HB2    | 1.71                     | 0.54              |
| 6:U:383:ARG:HH11  | 6:U:540:PRO:HD2   | 1.72                     | 0.54              |
| 1:L:775:VAL:HG11  | 1:L:928:LEU:H     | 1.73                     | 0.54              |
| 1:D:244:PHE:HA    | 1:D:247:ARG:HG2   | 1.88                     | 0.54              |
| 1:F:469:LEU:HD21  | 1:F:1143:ASN:HD22 | 1.72                     | 0.54              |
| 6:V:320:LEU:HB2   | 6:V:324:PRO:HG3   | 1.89                     | 0.54              |
| 1:B:1223:ASN:HD21 | 1:B:1228:ALA:H    | 1.54                     | 0.54              |
| 1:F:1178:PRO:HB2  | 1:F:1183:PRO:HD2  | 1.89                     | 0.54              |
| 1:J:1198:ARG:H    | 1:L:218:PRO:HG3   | 1.73                     | 0.54              |
| 1:J:1201:ALA:HB3  | 1:L:225:VAL:HB    | 1.90                     | 0.54              |
| 1:A:203:LYS:HE2   | 1:A:1124:GLY:HA2  | 1.89                     | 0.54              |
| 1:F:818:THR:HG23  | 1:F:819:PRO:HD3   | 1.90                     | 0.54              |
| 1:B:599:PRO:HB2   | 1:B:602:LEU:HD23  | 1.90                     | 0.53              |
| 1:F:90:ALA:HB1    | 1:F:1087:ARG:HA   | 1.89                     | 0.53              |
| 1:H:1291:PRO:HA   | 1:H:1294:LYS:HG2  | 1.89                     | 0.53              |
| 4:O:78:ILE:HG23   | 4:O:80:GLY:H      | 1.73                     | 0.53              |
| 5:T:146:GLU:HG3   | 5:T:361:ARG:HH21  | 1.73                     | 0.53              |
| 1:D:793:ASN:HD21  | 1:D:795:GLN:HB2   | 1.74                     | 0.53              |
| 1:L:500:ARG:HB3   | 1:L:567:VAL:HG11  | 1.90                     | 0.53              |
| 6:V:439:LEU:O     | 6:V:443:TYR:CB    | 2.55                     | 0.53              |
| 6:U:450:LEU:HB3   | 6:V:417:VAL:HA    | 1.90                     | 0.53              |
| 1:B:726:ILE:HG21  | 1:B:1060:ARG:HE   | 1.73                     | 0.53              |
| 1:D:475:MET:HA    | 1:D:1059:LEU:HG   | 1.90                     | 0.53              |
| 1:A:519:GLN:HE22  | 1:A:1012:PHE:HD2  | 1.54                     | 0.53              |
| 1:H:330:ALA:HA    | 1:H:334:GLY:H     | 1.74                     | 0.53              |
| 2:I:93:ARG:HB3    | 1:J:857:PRO:HG2   | 1.91                     | 0.53              |
| 1:H:427:GLN:HE21  | 1:H:433:ARG:HE    | 1.54                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:251:GLU:HB3   | 1:L:254:LEU:HB2   | 1.91                     | 0.53              |
| 1:B:872:GLU:HG2   | 1:B:874:PRO:HD3   | 1.91                     | 0.53              |
| 1:H:916:LEU:HD11  | 1:H:919:ASP:HB2   | 1.90                     | 0.53              |
| 1:J:152:LEU:O     | 1:J:156:SER:HB2   | 2.09                     | 0.53              |
| 6:V:321:PRO:HB2   | 6:V:322:PRO:HD3   | 1.90                     | 0.53              |
| 1:A:637:ARG:HA    | 1:A:959:MET:HE1   | 1.90                     | 0.53              |
| 4:O:29:LYS:HB3    | 4:O:74:ILE:HD12   | 1.90                     | 0.53              |
| 1:F:833:TYR:HA    | 1:F:837:ILE:HD12  | 1.91                     | 0.52              |
| 1:L:982:LEU:HD21  | 1:L:1022:ARG:HB2  | 1.89                     | 0.52              |
| 6:U:248:GLU:H     | 6:U:249:PRO:CD    | 2.18                     | 0.52              |
| 2:E:85:GLU:HA     | 2:E:90:THR:HG21   | 1.91                     | 0.52              |
| 1:L:205:PRO:HD2   | 1:L:207:LEU:HD23  | 1.90                     | 0.52              |
| 1:L:1157:MET:H    | 1:L:1159:HIS:HD2  | 1.56                     | 0.52              |
| 6:U:63:ALA:HB2    | 7:X:44:LEU:HD21   | 1.91                     | 0.52              |
| 1:D:892:ASN:H     | 2:G:98:LEU:HD13   | 1.74                     | 0.52              |
| 1:F:1285:ALA:HB1  | 1:F:1331:LYS:HG3  | 1.92                     | 0.52              |
| 4:O:140:ILE:HD11  | 4:O:144:LEU:HB2   | 1.90                     | 0.52              |
| 5:T:478:GLN:HA    | 5:T:640:GLY:HA3   | 1.90                     | 0.52              |
| 1:J:1241:ILE:HD12 | 1:J:1244:ILE:HD12 | 1.91                     | 0.52              |
| 1:J:506:VAL:HA    | 1:J:1015:ALA:HB2  | 1.90                     | 0.52              |
| 1:L:1301:VAL:HG23 | 1:L:1310:ARG:HH12 | 1.74                     | 0.52              |
| 6:U:316:ARG:HG3   | 6:U:317:LEU:HD12  | 1.91                     | 0.52              |
| 1:L:729:GLU:HG2   | 1:L:730:GLY:H     | 1.73                     | 0.52              |
| 3:N:404:ILE:HG21  | 4:O:227:LEU:HD21  | 1.91                     | 0.52              |
| 1:J:425:VAL:HG13  | 1:J:1215:LEU:HD21 | 1.92                     | 0.52              |
| 4:S:75:THR:HG22   | 4:S:76:ARG:H      | 1.74                     | 0.52              |
| 1:L:245:MET:HE2   | 1:L:259:LEU:HD22  | 1.91                     | 0.52              |
| 1:D:427:GLN:HB3   | 1:D:432:ASP:HB3   | 1.92                     | 0.52              |
| 1:H:1323:SER:HB2  | 1:H:1329:GLN:HA   | 1.91                     | 0.52              |
| 5:T:358:ILE:HG22  | 5:T:360:PRO:HD3   | 1.92                     | 0.52              |
| 1:D:508:VAL:HA    | 1:D:1011:PRO:HB2  | 1.92                     | 0.52              |
| 1:J:1194:ALA:HB3  | 1:J:1198:ARG:HD2  | 1.90                     | 0.52              |
| 2:K:10:VAL:HG11   | 2:K:36:LEU:HB3    | 1.92                     | 0.52              |
| 4:R:208:LEU:HD22  | 4:S:219:LEU:HB3   | 1.91                     | 0.51              |
| 1:H:905:VAL:HG11  | 1:H:909:ALA:H     | 1.75                     | 0.51              |
| 5:T:467:ILE:HG13  | 5:T:503:ILE:HD12  | 1.92                     | 0.51              |
| 6:U:384:ARG:HH21  | 6:U:540:PRO:HG2   | 1.74                     | 0.51              |
| 6:V:244:ASN:HD22  | 6:V:245:SER:H     | 1.58                     | 0.51              |
| 1:D:683:ASN:HB2   | 1:D:686:MET:HB2   | 1.92                     | 0.51              |
| 1:D:687:LEU:HD23  | 1:D:690:ILE:HD11  | 1.92                     | 0.51              |
| 1:L:1013:LEU:HD23 | 1:L:1022:ARG:HH12 | 1.76                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:P:224:PRO:HB2   | 4:P:227:LEU:HB2   | 1.92                     | 0.51              |
| 1:L:1184:ILE:HG22 | 1:L:1185:PHE:H    | 1.76                     | 0.51              |
| 1:J:766:ALA:HB1   | 1:J:769:ARG:HB2   | 1.92                     | 0.51              |
| 1:L:542:LEU:HD22  | 1:L:546:GLN:HB3   | 1.93                     | 0.51              |
| 4:P:72:ALA:HB1    | 4:P:87:ILE:HD13   | 1.91                     | 0.51              |
| 6:V:401:GLN:HG3   | 6:V:404:LEU:HG    | 1.92                     | 0.51              |
| 1:H:237:ARG:O     | 1:H:241:ASP:CB    | 2.59                     | 0.51              |
| 6:V:282:GLN:HG2   | 6:V:539:GLN:HE21  | 1.76                     | 0.51              |
| 1:B:538:VAL:HG21  | 1:B:1006:VAL:HG12 | 1.92                     | 0.51              |
| 5:T:153:ARG:HB2   | 5:T:358:ILE:HB    | 1.91                     | 0.51              |
| 6:U:292:GLN:HB2   | 6:U:354:LEU:HB3   | 1.92                     | 0.51              |
| 1:D:978:PRO:HB3   | 1:D:1010:PRO:HG3  | 1.93                     | 0.51              |
| 1:J:1341:GLN:HG3  | 1:J:1343:PRO:HD3  | 1.93                     | 0.51              |
| 6:V:229:PHE:HB3   | 6:V:448:TYR:HB2   | 1.92                     | 0.51              |
| 1:A:833:TYR:HA    | 1:A:837:ILE:HD13  | 1.92                     | 0.51              |
| 4:O:297:CYS:HB3   | 4:O:314:ILE:HG21  | 1.92                     | 0.51              |
| 4:R:155:ARG:HB3   | 4:R:191:LEU:HD11  | 1.92                     | 0.51              |
| 1:H:1333:PRO:HG2  | 1:H:1336:SER:HB3  | 1.93                     | 0.50              |
| 1:F:210:LEU:HD12  | 1:F:213:ILE:HD12  | 1.93                     | 0.50              |
| 2:G:22:GLU:HG3    | 2:G:67:ARG:HH11   | 1.77                     | 0.50              |
| 1:L:899:HIS:HA    | 1:L:902:HIS:HD2   | 1.76                     | 0.50              |
| 4:O:262:GLN:HB3   | 5:T:6:ALA:HA      | 1.94                     | 0.50              |
| 4:S:11:LEU:HD13   | 4:S:82:LEU:HD13   | 1.93                     | 0.50              |
| 1:D:1021:ILE:HG22 | 1:D:1025:VAL:HG23 | 1.93                     | 0.50              |
| 1:H:1147:ASN:HB3  | 1:H:1150:PHE:HB3  | 1.93                     | 0.50              |
| 1:J:1210:PRO:HG3  | 1:J:1262:ASN:HB3  | 1.92                     | 0.50              |
| 1:B:299:LEU:HD12  | 1:B:304:LEU:HD23  | 1.93                     | 0.50              |
| 4:S:211:SER:HG    | 4:S:277:TRP:CD1   | 2.27                     | 0.50              |
| 1:B:80:VAL:HG11   | 1:B:401:VAL:HA    | 1.92                     | 0.50              |
| 1:B:561:PRO:HG3   | 1:B:1264:TRP:HD1  | 1.76                     | 0.50              |
| 1:F:235:LYS:HG3   | 1:F:236:ARG:N     | 2.26                     | 0.50              |
| 3:Q:433:MET:HG3   | 3:Q:480:GLU:HB3   | 1.93                     | 0.50              |
| 6:U:378:ALA:HA    | 6:U:474:LEU:HD12  | 1.92                     | 0.50              |
| 1:B:535:PRO:HB2   | 1:B:538:VAL:HG22  | 1.94                     | 0.50              |
| 2:C:50:ILE:HB     | 2:C:54:ARG:HB2    | 1.92                     | 0.50              |
| 1:H:683:ASN:HB3   | 1:H:686:MET:HG2   | 1.93                     | 0.50              |
| 1:J:1012:PHE:HD1  | 1:J:1013:LEU:HD23 | 1.75                     | 0.50              |
| 1:A:186:ASP:HA    | 1:A:189:GLU:CD    | 2.37                     | 0.50              |
| 1:B:890:VAL:HG23  | 2:E:97:GLY:HA3    | 1.93                     | 0.50              |
| 1:F:874:PRO:HB2   | 1:F:882:HIS:HD2   | 1.76                     | 0.50              |
| 1:J:603:CYS:HB2   | 1:J:607:PHE:HB3   | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:O:223:ILE:HG13  | 4:O:224:PRO:HD3   | 1.94                     | 0.50              |
| 3:N:322:PHE:HD2   | 3:N:437:TYR:HB2   | 1.77                     | 0.50              |
| 4:O:219:LEU:HB3   | 4:P:213:ASN:HD21  | 1.76                     | 0.50              |
| 3:Q:480:GLU:H     | 4:R:283:ARG:HH22  | 1.60                     | 0.50              |
| 6:V:224:ARG:HH22  | 6:V:350:ALA:HB1   | 1.76                     | 0.50              |
| 1:A:190:ARG:HD2   | 1:A:401:VAL:HA    | 1.93                     | 0.49              |
| 1:A:421:MET:HE3   | 1:A:1355:CYS:HB3  | 1.94                     | 0.49              |
| 1:D:491:VAL:HG22  | 1:D:495:GLN:HE22  | 1.76                     | 0.49              |
| 1:H:526:THR:O     | 1:H:530:MET:HB3   | 2.12                     | 0.49              |
| 1:H:746:ASP:HB3   | 1:H:762:ARG:HE    | 1.76                     | 0.49              |
| 1:A:859:LEU:HG    | 1:A:917:MET:HE1   | 1.94                     | 0.49              |
| 1:F:841:SER:HB2   | 1:F:844:SER:HB3   | 1.94                     | 0.49              |
| 1:L:242:MET:HE1   | 1:L:1388:LEU:HB2  | 1.94                     | 0.49              |
| 1:L:1013:LEU:HG   | 1:L:1016:ASN:HB2  | 1.93                     | 0.49              |
| 6:V:236:LEU:HA    | 6:V:239:MET:HG2   | 1.94                     | 0.49              |
| 1:A:842:ARG:HG3   | 1:A:1039:LEU:HD11 | 1.94                     | 0.49              |
| 1:B:867:ILE:HD12  | 1:B:873:ALA:HB2   | 1.93                     | 0.49              |
| 1:H:1223:ASN:HD21 | 1:H:1348:GLN:HB3  | 1.77                     | 0.49              |
| 1:L:877:PRO:HG3   | 1:L:899:HIS:HB3   | 1.95                     | 0.49              |
| 6:V:105:ALA:O     | 6:V:108:GLU:HG3   | 2.13                     | 0.49              |
| 1:D:674:GLN:HG2   | 1:F:698:GLU:HG3   | 1.94                     | 0.49              |
| 1:L:701:GLU:HA    | 1:L:704:ILE:HG12  | 1.94                     | 0.49              |
| 6:V:94:ARG:HH11   | 6:V:98:VAL:HG21   | 1.77                     | 0.49              |
| 3:Q:346:ASN:HD21  | 3:Q:348:GLN:HB3   | 1.78                     | 0.49              |
| 4:R:144:LEU:O     | 4:R:147:GLU:HG3   | 2.13                     | 0.49              |
| 4:S:42:LEU:HD13   | 4:S:45:ILE:HD13   | 1.94                     | 0.49              |
| 6:V:80:GLU:HA     | 6:V:83:ARG:HD3    | 1.93                     | 0.49              |
| 1:A:526:THR:O     | 1:A:530:MET:HB2   | 2.13                     | 0.49              |
| 1:B:542:LEU:HD12  | 1:D:1060:ARG:HE   | 1.76                     | 0.49              |
| 1:F:1068:ALA:HB2  | 1:F:1211:VAL:HA   | 1.94                     | 0.49              |
| 1:H:555:LEU:HD23  | 1:H:1248:HIS:HB3  | 1.95                     | 0.49              |
| 3:N:393:ASP:HB2   | 3:N:394:PRO:HD3   | 1.94                     | 0.49              |
| 6:V:526:MET:HA    | 6:V:529:TYR:HD1   | 1.78                     | 0.49              |
| 1:F:665:THR:HG21  | 1:F:694:LEU:HD13  | 1.95                     | 0.49              |
| 3:Q:195:VAL:HG11  | 3:Q:274:ILE:HG21  | 1.94                     | 0.49              |
| 5:T:482:TYR:HE2   | 5:T:640:GLY:H     | 1.59                     | 0.49              |
| 6:V:338:ASN:HB2   | 6:V:456:LEU:HD23  | 1.94                     | 0.49              |
| 1:H:960:ALA:HA    | 1:H:987:GLU:HG3   | 1.95                     | 0.49              |
| 1:L:569:PRO:HG2   | 1:L:572:VAL:HG21  | 1.93                     | 0.49              |
| 3:N:317:GLY:HA2   | 4:O:36:LEU:HB3    | 1.95                     | 0.49              |
| 1:D:454:PRO:HG3   | 1:D:1379:GLN:HG3  | 1.95                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:488:ALA:HB3  | 1:D:1274:ARG:HH22 | 1.77                     | 0.49              |
| 1:J:741:ASN:HD22 | 1:J:744:THR:HB    | 1.78                     | 0.49              |
| 4:O:17:PRO:HA    | 4:O:20:THR:HB     | 1.95                     | 0.49              |
| 5:T:358:ILE:HG23 | 5:T:371:ILE:HG13  | 1.94                     | 0.49              |
| 1:H:270:VAL:HG12 | 1:H:1123:VAL:HG13 | 1.95                     | 0.48              |
| 1:L:801:LEU:HD13 | 1:L:922:GLU:HG3   | 1.95                     | 0.48              |
| 4:R:71:ALA:HB2   | 4:R:293:ILE:HD12  | 1.94                     | 0.48              |
| 1:A:990:ALA:HB1  | 1:A:1000:ARG:HE   | 1.78                     | 0.48              |
| 1:D:333:MET:HE2  | 1:D:335:LYS:HD2   | 1.95                     | 0.48              |
| 5:T:81:LEU:HD23  | 5:T:84:LEU:HD21   | 1.96                     | 0.48              |
| 6:U:450:LEU:H    | 6:V:417:VAL:HG12  | 1.78                     | 0.48              |
| 1:A:938:ALA:HA   | 1:A:943:ARG:HH21  | 1.78                     | 0.48              |
| 1:H:536:HIS:HA   | 1:H:539:ASN:HD21  | 1.78                     | 0.48              |
| 1:B:477:THR:HG21 | 1:B:1148:LEU:HB3  | 1.94                     | 0.48              |
| 1:F:981:PRO:HB3  | 1:F:1009:ILE:HG22 | 1.95                     | 0.48              |
| 1:H:465:ILE:HG22 | 1:J:1220:THR:HB   | 1.95                     | 0.48              |
| 1:L:1214:ASP:HB3 | 1:L:1217:TYR:HB3  | 1.94                     | 0.48              |
| 3:N:399:CYS:HB3  | 3:N:403:GLU:HB2   | 1.95                     | 0.48              |
| 6:U:229:PHE:HD2  | 6:U:464:VAL:HG13  | 1.77                     | 0.48              |
| 6:V:378:ALA:HB2  | 6:V:463:LEU:HD22  | 1.94                     | 0.48              |
| 1:A:210:LEU:HD12 | 1:A:213:ILE:HD13  | 1.94                     | 0.48              |
| 1:A:409:TYR:HB3  | 1:A:412:ILE:HG13  | 1.96                     | 0.48              |
| 1:D:1289:TYR:HB3 | 1:D:1291:PRO:HD2  | 1.95                     | 0.48              |
| 1:D:1081:GLN:HG2 | 1:D:1131:THR:HB   | 1.96                     | 0.48              |
| 1:J:141:LEU:HD21 | 1:J:188:PHE:HZ    | 1.78                     | 0.48              |
| 1:J:1361:MET:HE3 | 1:J:1379:GLN:HB3  | 1.95                     | 0.48              |
| 4:O:142:GLN:HA   | 4:O:145:MET:HB3   | 1.96                     | 0.48              |
| 4:S:11:LEU:HB2   | 4:S:82:LEU:HD22   | 1.95                     | 0.48              |
| 1:H:541:HIS:HD2  | 1:H:542:LEU:HD23  | 1.79                     | 0.48              |
| 1:L:962:GLN:HE21 | 1:L:967:THR:HB    | 1.78                     | 0.48              |
| 3:N:147:HIS:HD2  | 3:N:149:SER:HB2   | 1.78                     | 0.48              |
| 5:T:190:VAL:HA   | 5:T:193:MET:HE2   | 1.96                     | 0.48              |
| 6:U:447:LEU:HD12 | 6:U:448:TYR:HB2   | 1.96                     | 0.48              |
| 1:F:460:TYR:HB3  | 1:F:464:GLY:HA2   | 1.95                     | 0.48              |
| 6:U:452:ARG:HE   | 6:V:141:ALA:HB2   | 1.79                     | 0.48              |
| 1:D:174:ILE:O    | 1:D:177:MET:HG3   | 2.14                     | 0.48              |
| 1:L:889:LEU:HG   | 1:L:890:VAL:H     | 1.79                     | 0.48              |
| 3:N:258:PHE:HB3  | 4:P:295:ARG:HH22  | 1.79                     | 0.48              |
| 4:R:108:ASN:HD21 | 4:R:298:VAL:HG22  | 1.79                     | 0.48              |
| 6:U:56:LEU:HD13  | 6:V:56:LEU:HD11   | 1.95                     | 0.48              |
| 1:B:675:SER:HB2  | 1:B:677:ARG:HG2   | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:648:ALA:HB2   | 1:D:956:LEU:HD21  | 1.96                     | 0.48              |
| 1:J:556:ARG:HD2   | 1:J:1248:HIS:HD2  | 1.79                     | 0.48              |
| 4:S:100:ASN:HB3   | 4:S:307:PRO:HA    | 1.95                     | 0.48              |
| 5:T:182:ILE:HA    | 5:T:185:TYR:HD1   | 1.78                     | 0.48              |
| 1:A:205:PRO:HD2   | 1:A:1127:ALA:HB3  | 1.95                     | 0.47              |
| 4:O:104:VAL:HG12  | 4:O:183:ARG:HH12  | 1.79                     | 0.47              |
| 1:F:1049:LYS:HB3  | 1:F:1051:THR:HG22 | 1.95                     | 0.47              |
| 3:N:143:LEU:HD23  | 3:N:256:ILE:HG21  | 1.96                     | 0.47              |
| 1:A:1094:VAL:HG23 | 1:A:1116:ARG:HE   | 1.80                     | 0.47              |
| 1:H:741:ASN:HD22  | 1:H:744:THR:HG23  | 1.79                     | 0.47              |
| 1:J:650:ILE:HA    | 1:J:653:ASN:HB2   | 1.96                     | 0.47              |
| 2:M:87:ASP:HB3    | 2:M:90:THR:HG22   | 1.96                     | 0.47              |
| 4:O:29:LYS:HD2    | 4:O:29:LYS:HA     | 1.71                     | 0.47              |
| 1:D:155:LEU:HD13  | 1:D:158:THR:HG21  | 1.95                     | 0.47              |
| 1:D:702:VAL:HG23  | 1:D:703:CYS:H     | 1.80                     | 0.47              |
| 1:F:174:ILE:HA    | 1:F:177:MET:HG2   | 1.97                     | 0.47              |
| 1:H:144:ALA:HB3   | 1:J:124:VAL:HG21  | 1.96                     | 0.47              |
| 1:J:889:LEU:O     | 1:J:890:VAL:HG22  | 2.15                     | 0.47              |
| 1:J:1182:LEU:HD13 | 1:J:1188:LEU:HD13 | 1.95                     | 0.47              |
| 6:V:320:LEU:HD22  | 6:V:320:LEU:HA    | 1.75                     | 0.47              |
| 1:A:1051:THR:O    | 1:A:1055:LEU:HB2  | 2.15                     | 0.47              |
| 1:A:1218:PHE:HA   | 1:A:1222:CYS:HB3  | 1.96                     | 0.47              |
| 1:B:664:LEU:HD22  | 1:B:690:ILE:HD11  | 1.96                     | 0.47              |
| 1:L:200:LEU:HD11  | 1:L:1083:LEU:HB2  | 1.96                     | 0.47              |
| 1:A:747:THR:HA    | 1:A:762:ARG:HG3   | 1.96                     | 0.47              |
| 1:B:117:ALA:HB3   | 1:D:188:PHE:HA    | 1.95                     | 0.47              |
| 1:L:1145:ALA:HB3  | 1:L:1176:LEU:HD21 | 1.97                     | 0.47              |
| 6:V:115:GLN:O     | 6:V:118:GLU:HG3   | 2.15                     | 0.47              |
| 1:B:630:VAL:HG13  | 1:B:840:PHE:HE1   | 1.79                     | 0.47              |
| 1:F:857:PRO:HB2   | 2:G:54:ARG:HD2    | 1.97                     | 0.47              |
| 1:F:865:PRO:HG3   | 1:F:883:PRO:HG3   | 1.95                     | 0.47              |
| 1:H:952:LEU:HD21  | 1:H:955:GLY:HA3   | 1.96                     | 0.47              |
| 1:J:442:SER:HB3   | 1:L:436:ARG:HB2   | 1.97                     | 0.47              |
| 1:J:1147:ASN:HD21 | 1:J:1330:PHE:HE1  | 1.63                     | 0.47              |
| 3:N:262:LEU:H     | 3:N:262:LEU:HD23  | 1.80                     | 0.47              |
| 3:N:407:VAL:HG13  | 3:N:409:TRP:H     | 1.78                     | 0.47              |
| 3:Q:141:ILE:H     | 3:Q:299:ILE:HD11  | 1.80                     | 0.47              |
| 3:Q:173:ARG:HA    | 3:Q:173:ARG:HD2   | 1.71                     | 0.47              |
| 4:R:216:CYS:SG    | 4:S:213:ASN:HA    | 2.55                     | 0.47              |
| 6:U:415:ASN:HB3   | 6:U:436:PHE:HE1   | 1.80                     | 0.47              |
| 6:U:439:LEU:O     | 6:U:443:TYR:HB2   | 2.14                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:U:499:ILE:O    | 6:U:502:GLU:HG3   | 2.14                     | 0.47              |
| 6:V:226:TYR:HB2  | 6:V:337:ARG:HB3   | 1.96                     | 0.47              |
| 6:V:456:LEU:HA   | 6:V:459:MET:HB2   | 1.97                     | 0.47              |
| 6:V:550:ARG:HG2  | 6:V:553:ALA:HB2   | 1.96                     | 0.47              |
| 1:B:457:ILE:HD11 | 1:B:1355:CYS:HB2  | 1.95                     | 0.47              |
| 4:O:112:ILE:HA   | 4:O:141:PRO:HB3   | 1.97                     | 0.47              |
| 6:V:531:ARG:HB3  | 6:V:535:MET:HE2   | 1.97                     | 0.47              |
| 1:A:630:VAL:HA   | 1:A:633:THR:HG22  | 1.95                     | 0.47              |
| 1:B:890:VAL:HG21 | 2:E:95:THR:HG22   | 1.95                     | 0.47              |
| 1:L:283:ARG:HD2  | 1:L:391:LEU:HD22  | 1.96                     | 0.47              |
| 6:U:51:LEU:HA    | 6:U:54:ASN:HD21   | 1.80                     | 0.47              |
| 6:U:562:ASP:HA   | 6:U:565:TYR:HD1   | 1.80                     | 0.47              |
| 1:A:545:LEU:HD13 | 1:A:548:ILE:HD11  | 1.96                     | 0.47              |
| 1:B:421:MET:HE3  | 1:B:457:ILE:HG12  | 1.95                     | 0.47              |
| 1:D:497:HIS:HE1  | 1:D:585:PRO:HG2   | 1.78                     | 0.47              |
| 1:H:508:VAL:HG13 | 1:H:1014:GLY:HA3  | 1.97                     | 0.47              |
| 4:R:97:PHE:HD1   | 4:R:313:VAL:H     | 1.63                     | 0.47              |
| 1:B:227:ARG:HD3  | 1:B:1307:THR:HG21 | 1.96                     | 0.46              |
| 1:H:863:ILE:HD11 | 2:I:30:VAL:HG11   | 1.97                     | 0.46              |
| 6:U:239:MET:HG3  | 6:U:286:ASP:HB3   | 1.98                     | 0.46              |
| 6:V:468:LEU:HD22 | 6:V:495:LEU:HD11  | 1.97                     | 0.46              |
| 1:A:939:THR:HB   | 1:A:1157:MET:HE1  | 1.96                     | 0.46              |
| 1:J:209:LEU:HB3  | 1:J:234:LEU:HD22  | 1.96                     | 0.46              |
| 1:J:978:PRO:HD3  | 1:J:989:LEU:HD21  | 1.95                     | 0.46              |
| 1:F:831:ILE:HG23 | 1:F:835:ILE:HD12  | 1.97                     | 0.46              |
| 4:P:15:LEU:O     | 4:P:19:GLU:HB2    | 2.16                     | 0.46              |
| 6:U:416:ASN:C    | 6:U:418:ILE:H     | 2.23                     | 0.46              |
| 1:J:862:VAL:HB   | 1:J:917:MET:HE1   | 1.97                     | 0.46              |
| 1:L:500:ARG:HH12 | 1:L:553:PRO:HB3   | 1.80                     | 0.46              |
| 1:A:1036:PHE:HA  | 1:A:1039:LEU:HB2  | 1.97                     | 0.46              |
| 1:D:961:TYR:HB2  | 1:D:988:HIS:CE1   | 2.50                     | 0.46              |
| 1:F:526:THR:O    | 1:F:530:MET:CB    | 2.64                     | 0.46              |
| 1:F:1159:HIS:HB3 | 1:F:1162:VAL:HG22 | 1.96                     | 0.46              |
| 1:J:1366:HIS:HB2 | 1:L:1373:ASP:HB2  | 1.97                     | 0.46              |
| 3:N:262:LEU:HD12 | 3:N:274:ILE:HG21  | 1.96                     | 0.46              |
| 5:T:230:ARG:O    | 5:T:233:GLU:HG3   | 2.15                     | 0.46              |
| 1:D:889:LEU:O    | 1:D:890:VAL:HG22  | 2.16                     | 0.46              |
| 1:L:650:ILE:HG12 | 1:L:686:MET:HE3   | 1.97                     | 0.46              |
| 3:Q:195:VAL:HG21 | 3:Q:274:ILE:HG13  | 1.97                     | 0.46              |
| 1:A:1300:GLU:HA  | 1:A:1303:THR:HG22 | 1.98                     | 0.46              |
| 1:B:411:LEU:HD21 | 1:B:1081:GLN:HG3  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:917:MET:HA    | 1:B:920:MET:HE3   | 1.97                     | 0.46              |
| 1:F:503:TYR:HE1   | 1:F:567:VAL:HB    | 1.80                     | 0.46              |
| 1:F:1081:GLN:HA   | 1:F:1131:THR:HG21 | 1.98                     | 0.46              |
| 6:U:147:THR:HG21  | 6:U:166:ASN:HB3   | 1.97                     | 0.46              |
| 6:V:386:LEU:HD22  | 6:V:443:TYR:HE2   | 1.81                     | 0.46              |
| 1:B:434:TYR:HE2   | 1:D:1377:LEU:HD13 | 1.81                     | 0.46              |
| 1:F:830:LYS:O     | 1:F:834:TYR:HB2   | 2.15                     | 0.46              |
| 1:H:202:GLU:HB2   | 1:H:1316:LYS:HA   | 1.97                     | 0.46              |
| 1:H:600:VAL:N     | 1:H:601:PRO:HD3   | 2.31                     | 0.46              |
| 1:J:1199:GLY:H    | 1:L:226:ALA:HB1   | 1.80                     | 0.46              |
| 1:L:267:GLN:HE21  | 1:L:1125:TYR:HB3  | 1.79                     | 0.46              |
| 4:P:13:GLY:O      | 4:P:14:GLU:HG3    | 2.16                     | 0.46              |
| 6:V:261:LEU:O     | 6:V:265:THR:HB    | 2.16                     | 0.46              |
| 1:D:846:CYS:HB2   | 1:D:988:HIS:CD2   | 2.50                     | 0.46              |
| 1:F:80:VAL:HA     | 1:F:84:GLU:HG2    | 1.98                     | 0.46              |
| 1:F:1167:ARG:HE   | 1:F:1182:LEU:HD21 | 1.79                     | 0.46              |
| 1:J:757:ASP:HA    | 1:J:760:ILE:HD12  | 1.98                     | 0.46              |
| 1:L:174:ILE:HA    | 1:L:177:MET:HG2   | 1.98                     | 0.46              |
| 1:L:1180:GLU:HG3  | 1:L:1181:PRO:HD3  | 1.98                     | 0.46              |
| 1:A:972:THR:HG23  | 6:U:536:LEU:HD11  | 1.98                     | 0.46              |
| 1:D:1161:ASN:O    | 1:D:1164:GLU:HG3  | 2.16                     | 0.46              |
| 1:L:753:LEU:HB2   | 1:L:953:TYR:HE1   | 1.81                     | 0.46              |
| 1:B:548:ILE:HA    | 1:B:1259:ALA:HB2  | 1.98                     | 0.45              |
| 1:B:989:LEU:HB3   | 1:B:995:MET:HE1   | 1.97                     | 0.45              |
| 5:T:80:ALA:HA     | 5:T:83:ASN:HD21   | 1.81                     | 0.45              |
| 1:F:787:VAL:HG11  | 1:F:796:ARG:HH12  | 1.81                     | 0.45              |
| 1:F:805:ARG:HA    | 1:F:818:THR:HG21  | 1.97                     | 0.45              |
| 1:H:692:THR:HG21  | 1:J:964:TYR:HB2   | 1.98                     | 0.45              |
| 6:U:170:ILE:HG23  | 6:U:465:ALA:HB1   | 1.99                     | 0.45              |
| 6:U:177:ARG:HH21  | 6:U:578:THR:HB    | 1.81                     | 0.45              |
| 6:V:83:ARG:HE     | 6:V:84:ARG:HH12   | 1.64                     | 0.45              |
| 1:A:799:ASN:H     | 1:A:925:THR:HG21  | 1.81                     | 0.45              |
| 1:B:248:HIS:CD2   | 1:B:250:ARG:H     | 2.34                     | 0.45              |
| 1:D:1250:GLN:CD   | 1:D:1251:SER:H    | 2.24                     | 0.45              |
| 1:F:1332:ARG:HH21 | 3:Q:270:ASN:HD21  | 1.63                     | 0.45              |
| 1:H:865:PRO:HB3   | 1:H:883:PRO:HG3   | 1.99                     | 0.45              |
| 1:J:583:ALA:HB2   | 5:T:575:LEU:HD22  | 1.99                     | 0.45              |
| 1:J:846:CYS:HB2   | 1:J:985:CYS:HB3   | 1.74                     | 0.45              |
| 3:N:140:SER:HA    | 3:N:198:LEU:HD22  | 1.99                     | 0.45              |
| 4:P:295:ARG:HA    | 4:P:295:ARG:HD2   | 1.74                     | 0.45              |
| 4:S:10:LEU:HD23   | 4:S:39:ARG:HH21   | 1.81                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:V:85:LEU:HD13   | 7:X:23:ARG:HG2    | 1.99                     | 0.45              |
| 1:H:1140:ASP:HB2  | 1:H:1199:GLY:HA3  | 1.98                     | 0.45              |
| 6:U:234:LEU:HA    | 6:U:237:TYR:HD1   | 1.82                     | 0.45              |
| 1:D:503:TYR:HB3   | 1:D:569:PRO:HG3   | 1.97                     | 0.45              |
| 1:H:407:VAL:HG13  | 1:J:116:ILE:HD13  | 1.99                     | 0.45              |
| 1:J:465:ILE:HG12  | 1:L:1216:GLN:HE22 | 1.80                     | 0.45              |
| 1:A:183:THR:HA    | 1:A:186:ASP:OD2   | 2.17                     | 0.45              |
| 1:A:475:MET:O     | 1:A:479:CYS:HB2   | 2.16                     | 0.45              |
| 1:A:1086:GLU:CD   | 1:A:1087:ARG:H    | 2.25                     | 0.45              |
| 1:H:701:GLU:HG3   | 1:J:677:ARG:HH22  | 1.82                     | 0.45              |
| 1:L:457:ILE:HG23  | 1:L:1356:SER:H    | 1.82                     | 0.45              |
| 6:U:226:TYR:HB2   | 6:V:411:GLY:HA2   | 1.98                     | 0.45              |
| 1:D:421:MET:HG2   | 1:D:457:ILE:HG21  | 1.99                     | 0.45              |
| 1:H:838:PRO:O     | 1:H:842:ARG:HB3   | 2.16                     | 0.45              |
| 4:S:207:ASN:HA    | 4:S:210:PHE:HD1   | 1.82                     | 0.45              |
| 5:T:476:LEU:O     | 5:T:477:GLN:HG3   | 2.16                     | 0.45              |
| 6:U:239:MET:HE3   | 6:U:239:MET:HB3   | 1.82                     | 0.45              |
| 1:L:1114:GLN:HB3  | 1:L:1116:ARG:HE   | 1.82                     | 0.45              |
| 6:U:278:LYS:HD3   | 6:U:428:LYS:HB3   | 1.97                     | 0.45              |
| 6:U:481:ARG:HB3   | 6:U:483:VAL:HG22  | 1.99                     | 0.45              |
| 6:V:315:ILE:HG22  | 6:V:319:VAL:HG12  | 1.99                     | 0.45              |
| 1:A:595:ASN:HD21  | 1:A:1049:LYS:HA   | 1.81                     | 0.45              |
| 1:A:1140:ASP:HB2  | 1:A:1202:SER:HB2  | 1.99                     | 0.45              |
| 1:H:939:THR:HG23  | 1:H:942:THR:H     | 1.82                     | 0.45              |
| 3:N:444:PRO:HD3   | 3:N:471:VAL:HG22  | 1.99                     | 0.45              |
| 4:P:61:SER:O      | 4:P:64:GLU:HG3    | 2.16                     | 0.45              |
| 4:P:78:ILE:HG22   | 4:P:80:GLY:H      | 1.82                     | 0.45              |
| 6:U:380:LEU:HD11  | 6:U:537:MET:HG3   | 1.99                     | 0.45              |
| 1:B:833:TYR:HD1   | 1:B:837:ILE:HD12  | 1.82                     | 0.45              |
| 1:F:411:LEU:HB3   | 1:F:1081:GLN:HB3  | 1.99                     | 0.45              |
| 6:U:51:LEU:HA     | 6:U:54:ASN:ND2    | 2.32                     | 0.45              |
| 1:A:1101:HIS:HB3  | 1:A:1110:PHE:HB3  | 1.99                     | 0.44              |
| 1:D:1240:ASP:O    | 1:D:1241:ILE:HG22 | 2.18                     | 0.44              |
| 1:F:171:ILE:HA    | 1:F:174:ILE:HG12  | 1.99                     | 0.44              |
| 1:H:1087:ARG:HH21 | 1:H:1124:GLY:HA3  | 1.83                     | 0.44              |
| 1:J:1173:GLY:HA3  | 1:L:1251:SER:HB2  | 1.99                     | 0.44              |
| 1:J:1321:GLN:HA   | 1:J:1332:ARG:HB2  | 1.98                     | 0.44              |
| 4:S:59:THR:HG23   | 4:S:118:VAL:HG11  | 1.98                     | 0.44              |
| 5:T:26:VAL:HB     | 5:T:371:ILE:HG23  | 1.98                     | 0.44              |
| 6:U:138:LYS:HE3   | 6:U:414:THR:HA    | 1.99                     | 0.44              |
| 1:A:517:ASP:O     | 1:A:520:MET:HG2   | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:196:LEU:HD12  | 1:B:1116:ARG:HH12 | 1.82                     | 0.44              |
| 1:H:549:ALA:N     | 1:H:550:PRO:HD2   | 2.32                     | 0.44              |
| 1:J:594:ILE:HD12  | 1:J:1020:THR:H    | 1.81                     | 0.44              |
| 1:L:914:GLN:HG2   | 2:M:65:ALA:HB1    | 1.99                     | 0.44              |
| 1:L:1364:THR:HB   | 1:L:1368:GLY:HA2  | 1.99                     | 0.44              |
| 1:A:725:THR:HG21  | 1:A:740:ASN:HA    | 1.98                     | 0.44              |
| 2:E:92:LEU:HD23   | 2:E:92:LEU:HA     | 1.88                     | 0.44              |
| 1:J:608:ARG:O     | 1:J:611:ARG:HG3   | 2.17                     | 0.44              |
| 1:L:1180:GLU:N    | 1:L:1181:PRO:HD2  | 2.33                     | 0.44              |
| 1:F:537:TRP:HB2   | 1:F:554:ARG:HH21  | 1.83                     | 0.44              |
| 1:J:1057:HIS:HA   | 1:J:1060:ARG:HG2  | 1.99                     | 0.44              |
| 1:J:1176:LEU:HD13 | 1:L:1244:ILE:HA   | 1.99                     | 0.44              |
| 2:K:98:LEU:HD13   | 1:L:896:VAL:HG21  | 1.98                     | 0.44              |
| 3:Q:237:ARG:O     | 3:Q:240:GLU:HG3   | 2.17                     | 0.44              |
| 7:X:11:ALA:O      | 7:X:14:ARG:HG3    | 2.18                     | 0.44              |
| 2:C:9:VAL:HG12    | 2:C:11:PHE:H      | 1.83                     | 0.44              |
| 1:F:598:ILE:N     | 1:F:599:PRO:HD2   | 2.33                     | 0.44              |
| 5:T:242:ILE:HD12  | 6:V:94:ARG:HE     | 1.82                     | 0.44              |
| 6:U:522:HIS:HA    | 6:U:525:VAL:HB    | 1.99                     | 0.44              |
| 1:A:653:ASN:HB3   | 1:A:656:ASN:HB2   | 2.00                     | 0.44              |
| 4:P:33:PHE:HD1    | 4:P:45:ILE:HG21   | 1.81                     | 0.44              |
| 1:A:850:VAL:HG12  | 1:A:956:LEU:HD22  | 1.99                     | 0.44              |
| 1:D:502:CYS:HA    | 1:D:532:PRO:HG2   | 1.99                     | 0.44              |
| 1:H:471:LEU:HD23  | 1:H:475:MET:HG2   | 2.00                     | 0.44              |
| 4:R:138:LEU:HD23  | 4:R:140:ILE:HD11  | 1.99                     | 0.44              |
| 1:A:424:GLY:O     | 1:A:425:VAL:HG12  | 2.18                     | 0.44              |
| 1:B:846:CYS:HB3   | 1:B:988:HIS:CE1   | 2.53                     | 0.44              |
| 1:D:555:LEU:HD23  | 1:D:555:LEU:H     | 1.82                     | 0.44              |
| 1:D:660:LEU:HD22  | 1:D:912:THR:HB    | 2.00                     | 0.44              |
| 1:D:732:ASN:HD21  | 1:D:768:ASP:HB3   | 1.82                     | 0.44              |
| 1:F:48:PHE:HD1    | 1:F:48:PHE:HA     | 1.72                     | 0.44              |
| 1:F:520:MET:HE1   | 1:F:977:VAL:HG12  | 1.99                     | 0.44              |
| 1:F:526:THR:O     | 1:F:530:MET:HB2   | 2.18                     | 0.44              |
| 1:H:688:MET:HE2   | 1:H:688:MET:HB2   | 1.92                     | 0.44              |
| 1:L:247:ARG:HD3   | 1:L:1134:LEU:HD13 | 1.99                     | 0.44              |
| 1:L:831:ILE:HA    | 1:L:835:ILE:HD12  | 2.00                     | 0.44              |
| 6:U:167:SER:O     | 6:U:168:PRO:C     | 2.60                     | 0.44              |
| 1:H:759:LEU:O     | 1:H:762:ARG:HG3   | 2.18                     | 0.44              |
| 1:J:1349:GLU:H    | 1:J:1349:GLU:HG3  | 1.59                     | 0.44              |
| 3:N:343:SER:HB3   | 3:N:350:PHE:HE1   | 1.83                     | 0.44              |
| 4:O:145:MET:O     | 4:O:149:ILE:HG12  | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:R:47:LEU:O      | 4:R:51:TYR:HB2    | 2.18                     | 0.44              |
| 4:S:106:LEU:H     | 4:S:305:VAL:HG21  | 1.82                     | 0.44              |
| 1:A:640:PRO:HB2   | 1:A:643:PHE:HB2   | 2.00                     | 0.43              |
| 1:F:82:PHE:HB3    | 1:F:83:LEU:H      | 1.70                     | 0.43              |
| 1:F:335:LYS:HA    | 1:F:335:LYS:HD2   | 1.89                     | 0.43              |
| 1:H:475:MET:HE1   | 1:H:1060:ARG:HB2  | 2.00                     | 0.43              |
| 1:H:506:VAL:HA    | 1:H:1018:HIS:NE2  | 2.33                     | 0.43              |
| 1:J:1361:MET:HA   | 1:J:1376:HIS:HE1  | 1.82                     | 0.43              |
| 5:T:446:ALA:HA    | 5:T:449:PHE:CE2   | 2.53                     | 0.43              |
| 6:V:510:VAL:O     | 6:V:511:THR:HG22  | 2.18                     | 0.43              |
| 1:A:209:LEU:HB2   | 1:A:234:LEU:HD11  | 2.00                     | 0.43              |
| 2:G:17:THR:HG23   | 2:G:18:THR:H      | 1.82                     | 0.43              |
| 1:J:1326:THR:HG23 | 1:J:1328:TYR:H    | 1.83                     | 0.43              |
| 1:J:1363:ARG:HB3  | 1:L:1374:GLU:HG2  | 2.00                     | 0.43              |
| 6:V:184:VAL:HA    | 6:V:188:PRO:HB3   | 2.00                     | 0.43              |
| 1:A:637:ARG:HH21  | 1:A:962:GLN:HB3   | 1.82                     | 0.43              |
| 1:D:1076:ARG:HE   | 1:D:1138:LEU:HD22 | 1.84                     | 0.43              |
| 1:D:1258:ARG:HH12 | 1:D:1261:LEU:HD12 | 1.82                     | 0.43              |
| 4:R:148:ILE:HD13  | 4:R:148:ILE:HA    | 1.90                     | 0.43              |
| 5:T:586:LYS:H     | 5:T:586:LYS:HG3   | 1.75                     | 0.43              |
| 6:U:313:ALA:HA    | 6:U:316:ARG:HG2   | 2.00                     | 0.43              |
| 1:A:1156:PRO:HG3  | 4:O:236:VAL:HB    | 2.00                     | 0.43              |
| 1:B:721:ILE:HA    | 1:B:724:PHE:HD2   | 1.84                     | 0.43              |
| 1:B:889:LEU:HD12  | 1:B:889:LEU:HA    | 1.79                     | 0.43              |
| 1:F:542:LEU:HA    | 1:F:546:GLN:HB2   | 2.00                     | 0.43              |
| 1:L:430:SER:HA    | 1:L:433:ARG:HH22  | 1.83                     | 0.43              |
| 1:L:961:TYR:HB2   | 1:L:988:HIS:NE2   | 2.33                     | 0.43              |
| 6:U:566:PHE:HA    | 6:U:572:ILE:HD11  | 2.00                     | 0.43              |
| 6:V:390:ASN:O     | 6:V:391:VAL:HG12  | 2.18                     | 0.43              |
| 1:B:118:ARG:HA    | 1:D:193:ALA:H     | 1.84                     | 0.43              |
| 1:H:205:PRO:HD2   | 1:H:1127:ALA:HB1  | 1.99                     | 0.43              |
| 1:L:863:ILE:HD12  | 2:M:27:TYR:HB2    | 1.99                     | 0.43              |
| 4:O:253:ILE:HG13  | 4:O:254:ASN:H     | 1.84                     | 0.43              |
| 5:T:166:LYS:HD2   | 5:T:204:ILE:HG23  | 2.00                     | 0.43              |
| 5:T:546:TYR:HD2   | 5:T:547:LEU:HG    | 1.83                     | 0.43              |
| 1:B:118:ARG:N     | 1:D:192:THR:H     | 2.16                     | 0.43              |
| 1:F:169:LEU:O     | 1:F:172:ARG:HG2   | 2.18                     | 0.43              |
| 1:F:1200:GLN:HG3  | 1:F:1327:GLU:HA   | 2.01                     | 0.43              |
| 1:H:242:MET:HG2   | 1:H:243:PHE:HD1   | 1.83                     | 0.43              |
| 1:H:296:LYS:HD3   | 1:H:394:LEU:HD21  | 2.00                     | 0.43              |
| 1:H:1080:GLU:HG2  | 1:H:1135:ARG:HG2  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:1102:HIS:HB2  | 1:J:1111:THR:HG22 | 2.00                     | 0.43              |
| 1:B:935:ALA:HB2   | 1:B:943:ARG:HD2   | 2.01                     | 0.43              |
| 1:L:233:ASP:HA    | 1:L:236:ARG:HE    | 1.84                     | 0.43              |
| 1:L:251:GLU:HG2   | 1:L:254:LEU:HD12  | 2.00                     | 0.43              |
| 1:L:664:LEU:HD23  | 1:L:664:LEU:HA    | 1.90                     | 0.43              |
| 1:A:1210:PRO:HG3  | 1:A:1264:TRP:HB2  | 2.01                     | 0.43              |
| 1:B:399:ARG:HG3   | 1:B:401:VAL:HG22  | 2.00                     | 0.43              |
| 1:F:253:ARG:HD2   | 1:F:253:ARG:HA    | 1.83                     | 0.43              |
| 1:F:1262:ASN:HB2  | 1:F:1265:ALA:HB3  | 2.00                     | 0.43              |
| 1:H:237:ARG:O     | 1:H:241:ASP:HB3   | 2.19                     | 0.43              |
| 1:H:517:ASP:HA    | 1:H:520:MET:HE3   | 2.01                     | 0.43              |
| 1:J:523:PHE:HB2   | 1:J:1012:PHE:HE2  | 1.83                     | 0.43              |
| 1:J:647:GLU:HA    | 1:J:650:ILE:HG22  | 1.99                     | 0.43              |
| 4:P:206:LEU:O     | 4:P:209:MET:HG3   | 2.18                     | 0.43              |
| 6:U:108:GLU:HA    | 6:U:111:GLU:CD    | 2.44                     | 0.43              |
| 6:V:103:GLU:HB2   | 7:X:5:LEU:HB3     | 2.01                     | 0.43              |
| 1:A:631:LYS:HD3   | 1:A:631:LYS:HA    | 1.77                     | 0.43              |
| 1:A:1214:ASP:HB2  | 1:A:1261:LEU:HG   | 1.99                     | 0.43              |
| 1:B:611:ARG:HH12  | 1:B:1038:THR:HG22 | 1.84                     | 0.43              |
| 1:B:805:ARG:HA    | 1:B:805:ARG:HD2   | 1.85                     | 0.43              |
| 1:B:964:TYR:HD1   | 1:B:964:TYR:HA    | 1.76                     | 0.43              |
| 1:J:160:VAL:HG23  | 1:J:161:ASP:H     | 1.83                     | 0.43              |
| 1:J:985:CYS:HB2   | 1:J:988:HIS:HB2   | 2.00                     | 0.43              |
| 1:J:1100:HIS:HB3  | 1:J:1111:THR:HG23 | 2.00                     | 0.43              |
| 1:J:1121:LEU:HD12 | 1:J:1123:VAL:H    | 1.84                     | 0.43              |
| 1:L:457:ILE:HD12  | 1:L:1355:CYS:HB2  | 2.00                     | 0.43              |
| 1:L:1328:TYR:O    | 1:L:1329:GLN:HG3  | 2.19                     | 0.43              |
| 1:A:95:LYS:HD2    | 1:A:95:LYS:HA     | 1.86                     | 0.43              |
| 1:A:169:LEU:HD12  | 1:A:172:ARG:HE    | 1.84                     | 0.43              |
| 1:A:641:THR:HG23  | 1:A:956:LEU:HD21  | 2.01                     | 0.43              |
| 1:A:1166:LEU:HD23 | 1:A:1169:ILE:HD11 | 2.01                     | 0.43              |
| 1:B:623:THR:HG23  | 1:B:626:THR:H     | 1.84                     | 0.43              |
| 1:D:549:ALA:N     | 1:D:550:PRO:HD2   | 2.34                     | 0.43              |
| 1:H:1237:ARG:HG2  | 1:H:1239:ALA:H    | 1.84                     | 0.43              |
| 2:I:82:MET:H      | 2:I:82:MET:HG2    | 1.65                     | 0.43              |
| 4:P:168:PRO:HG3   | 5:T:336:ILE:HG12  | 2.01                     | 0.43              |
| 4:R:16:SER:H      | 4:R:17:PRO:HD2    | 1.84                     | 0.43              |
| 5:T:66:GLU:HG3    | 5:T:67:PRO:HD2    | 2.01                     | 0.43              |
| 6:U:274:THR:HG22  | 6:U:276:GLU:H     | 1.84                     | 0.43              |
| 6:V:135:GLN:HE21  | 6:V:402:LEU:HB3   | 1.83                     | 0.43              |
| 6:V:179:LEU:HD11  | 6:V:495:LEU:HB3   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:259:LEU:O     | 1:A:262:MET:HG2   | 2.19                     | 0.42              |
| 1:B:789:MET:HA    | 1:B:792:HIS:HD2   | 1.83                     | 0.42              |
| 1:H:939:THR:HG23  | 1:H:941:THR:H     | 1.84                     | 0.42              |
| 1:H:1290:SER:N    | 1:H:1291:PRO:HD2  | 2.34                     | 0.42              |
| 1:J:235:LYS:HE2   | 1:J:1349:GLU:HB3  | 2.01                     | 0.42              |
| 1:J:591:LEU:HD23  | 1:J:591:LEU:HA    | 1.88                     | 0.42              |
| 1:J:1222:CYS:HB2  | 1:J:1350:ALA:HB3  | 2.00                     | 0.42              |
| 1:L:205:PRO:HB2   | 1:L:206:PRO:HD2   | 2.01                     | 0.42              |
| 1:L:1059:LEU:HG   | 1:L:1063:PHE:HE2  | 1.83                     | 0.42              |
| 1:L:1097:ILE:HD12 | 1:L:1114:GLN:HB2  | 2.01                     | 0.42              |
| 3:N:416:LEU:HB3   | 3:N:417:TYR:H     | 1.55                     | 0.42              |
| 5:T:57:THR:HG22   | 5:T:66:GLU:H      | 1.83                     | 0.42              |
| 6:U:542:VAL:HG12  | 6:U:545:ALA:HB3   | 2.01                     | 0.42              |
| 1:A:429:ASN:HD21  | 1:A:603:CYS:HA    | 1.84                     | 0.42              |
| 1:B:500:ARG:HD2   | 1:B:500:ARG:HA    | 1.88                     | 0.42              |
| 1:B:1080:GLU:H    | 1:B:1135:ARG:HG3  | 1.83                     | 0.42              |
| 1:D:95:LYS:HG3    | 1:D:97:PRO:HD3    | 2.00                     | 0.42              |
| 1:D:245:MET:HG2   | 1:D:246:THR:HG23  | 2.00                     | 0.42              |
| 2:E:22:GLU:HG2    | 2:E:67:ARG:HD2    | 2.01                     | 0.42              |
| 1:J:1365:ALA:HB2  | 1:L:1376:HIS:HB2  | 2.01                     | 0.42              |
| 1:L:210:LEU:HD11  | 1:L:1308:LEU:HD22 | 2.00                     | 0.42              |
| 1:L:245:MET:HE3   | 1:L:245:MET:HB3   | 1.82                     | 0.42              |
| 4:O:119:PHE:HE1   | 4:O:185:TYR:HB3   | 1.83                     | 0.42              |
| 3:Q:171:GLY:HA2   | 3:Q:174:ASN:ND2   | 2.34                     | 0.42              |
| 3:Q:171:GLY:HA2   | 3:Q:174:ASN:HD21  | 1.83                     | 0.42              |
| 4:S:51:TYR:HB3    | 4:S:56:PRO:HG3    | 2.01                     | 0.42              |
| 4:S:219:LEU:O     | 4:S:223:ILE:HB    | 2.19                     | 0.42              |
| 5:T:4:HIS:O       | 5:T:8:GLU:HG2     | 2.18                     | 0.42              |
| 1:A:522:ARG:O     | 1:A:525:GLU:HG3   | 2.19                     | 0.42              |
| 1:B:116:ILE:HA    | 1:D:191:GLY:HA3   | 2.01                     | 0.42              |
| 1:D:326:ASN:HA    | 1:D:329:THR:HG22  | 1.99                     | 0.42              |
| 1:H:739:LEU:HD13  | 1:H:1049:LYS:HZ1  | 1.83                     | 0.42              |
| 1:L:222:LEU:HD12  | 1:L:226:ALA:HB2   | 2.01                     | 0.42              |
| 1:L:600:VAL:N     | 1:L:601:PRO:HD2   | 2.34                     | 0.42              |
| 1:L:998:ALA:HA    | 1:L:1001:VAL:HG22 | 1.99                     | 0.42              |
| 3:N:178:ALA:HB2   | 3:N:237:ARG:HD2   | 2.02                     | 0.42              |
| 1:A:304:LEU:HD13  | 1:A:385:VAL:HG21  | 2.01                     | 0.42              |
| 1:A:707:TYR:HA    | 1:A:710:LEU:HD23  | 2.01                     | 0.42              |
| 1:B:214:ASN:HA    | 1:B:217:GLN:HE22  | 1.84                     | 0.42              |
| 1:J:1176:LEU:O    | 1:L:1250:GLN:HB3  | 2.19                     | 0.42              |
| 1:L:466:LEU:HD13  | 1:L:1359:ALA:HB1  | 2.00                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:R:12:PRO:HB2   | 4:R:15:LEU:HD21   | 2.01                     | 0.42              |
| 6:U:129:SER:O    | 6:U:130:ILE:HG22  | 2.20                     | 0.42              |
| 6:U:434:ASN:HA   | 6:U:437:GLN:HE21  | 1.83                     | 0.42              |
| 6:V:346:ILE:HD12 | 6:V:349:ALA:HB3   | 2.01                     | 0.42              |
| 6:V:527:LEU:HD13 | 6:V:531:ARG:HH22  | 1.84                     | 0.42              |
| 1:D:685:HIS:HA   | 1:D:688:MET:HE3   | 2.02                     | 0.42              |
| 1:D:832:TYR:O    | 1:D:836:VAL:HG22  | 2.19                     | 0.42              |
| 1:L:253:ARG:HA   | 1:L:257:ALA:HB2   | 2.01                     | 0.42              |
| 6:V:133:GLU:HB3  | 6:V:142:PRO:HB2   | 2.01                     | 0.42              |
| 1:B:1010:PRO:HG2 | 1:B:1013:LEU:HD12 | 2.00                     | 0.42              |
| 3:N:141:ILE:HB   | 3:N:198:LEU:HD13  | 2.01                     | 0.42              |
| 6:U:192:ARG:HD2  | 6:U:192:ARG:HA    | 1.86                     | 0.42              |
| 6:V:135:GLN:HG2  | 6:V:402:LEU:HD12  | 2.01                     | 0.42              |
| 1:A:907:GLY:HA2  | 1:A:910:LEU:HD12  | 2.01                     | 0.42              |
| 1:B:406:ARG:HD2  | 1:B:406:ARG:HA    | 1.88                     | 0.42              |
| 1:B:857:PRO:HA   | 1:B:860:GLN:HE22  | 1.85                     | 0.42              |
| 2:K:32:LEU:O     | 2:K:36:LEU:HB2    | 2.20                     | 0.42              |
| 5:T:165:CYS:HA   | 5:T:168:LEU:HD23  | 2.01                     | 0.42              |
| 1:A:729:GLU:HB2  | 1:A:739:LEU:HD11  | 2.01                     | 0.42              |
| 1:A:959:MET:HG3  | 1:A:960:ALA:H     | 1.83                     | 0.42              |
| 1:B:44:HIS:O     | 1:B:45:ARG:HG2    | 2.20                     | 0.42              |
| 1:J:430:SER:HB3  | 1:J:433:ARG:HH22  | 1.85                     | 0.42              |
| 1:J:981:PRO:HB3  | 1:J:1009:ILE:HG23 | 2.01                     | 0.42              |
| 5:T:400:ASP:HB3  | 7:W:35:GLN:NE2    | 2.34                     | 0.42              |
| 6:V:103:GLU:HA   | 7:X:5:LEU:HD22    | 2.00                     | 0.42              |
| 1:A:288:VAL:HG23 | 1:A:1085:ALA:HB3  | 2.01                     | 0.42              |
| 1:J:990:ALA:HA   | 1:J:1000:ARG:HD3  | 2.02                     | 0.42              |
| 3:N:311:LEU:HD12 | 3:N:311:LEU:HA    | 1.87                     | 0.42              |
| 4:R:277:TRP:CE2  | 4:S:212:ILE:HG12  | 2.55                     | 0.42              |
| 5:T:384:ARG:HG2  | 5:T:389:PRO:HG3   | 2.02                     | 0.42              |
| 5:T:637:LEU:HD12 | 5:T:638:PRO:HD2   | 2.02                     | 0.42              |
| 1:A:559:LEU:HD23 | 1:A:559:LEU:HA    | 1.84                     | 0.42              |
| 1:D:962:GLN:HB2  | 1:D:965:ASP:HB2   | 2.02                     | 0.42              |
| 1:F:509:ALA:HB3  | 1:F:1011:PRO:HB2  | 2.01                     | 0.42              |
| 1:F:922:GLU:H    | 1:F:922:GLU:HG3   | 1.58                     | 0.42              |
| 1:H:1333:PRO:HA  | 1:H:1334:PRO:HD3  | 1.94                     | 0.42              |
| 1:J:654:GLU:HA   | 1:J:657:PHE:HB3   | 2.02                     | 0.42              |
| 1:J:1352:PRO:HA  | 1:J:1353:PRO:HD3  | 1.89                     | 0.42              |
| 1:L:1017:HIS:CD2 | 1:L:1022:ARG:HH21 | 2.38                     | 0.42              |
| 1:L:1087:ARG:H   | 1:L:1087:ARG:HG2  | 1.67                     | 0.42              |
| 6:V:131:HIS:HB3  | 6:V:144:GLN:HE22  | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:V:538:HIS:ND1   | 6:V:540:PRO:HD2   | 2.35                     | 0.42              |
| 1:A:726:ILE:H     | 1:A:1057:HIS:CD2  | 2.38                     | 0.41              |
| 1:A:874:PRO:HB2   | 1:A:876:THR:HG22  | 2.02                     | 0.41              |
| 1:A:1092:TYR:HD1  | 1:A:1118:HIS:HB3  | 1.85                     | 0.41              |
| 1:B:1010:PRO:HB2  | 1:B:1013:LEU:HB2  | 2.02                     | 0.41              |
| 1:L:19:ILE:HB     | 1:L:20:ALA:H      | 1.73                     | 0.41              |
| 1:L:838:PRO:HG3   | 1:L:983:PHE:HZ    | 1.84                     | 0.41              |
| 4:S:87:ILE:HG22   | 4:S:92:PRO:HA     | 2.02                     | 0.41              |
| 6:U:91:GLN:HB3    | 7:X:14:ARG:CZ     | 2.50                     | 0.41              |
| 1:A:285:VAL:HG21  | 1:A:393:PHE:HD1   | 1.85                     | 0.41              |
| 1:A:1356:SER:HB3  | 1:A:1362:LEU:HD12 | 2.02                     | 0.41              |
| 1:D:611:ARG:HH22  | 1:D:1058:GLN:HE22 | 1.68                     | 0.41              |
| 1:L:232:SER:HA    | 1:L:235:LYS:HG2   | 2.03                     | 0.41              |
| 4:O:108:ASN:HB2   | 4:O:303:SER:HB2   | 2.02                     | 0.41              |
| 6:U:289:PRO:HD2   | 6:U:376:ILE:HD11  | 2.02                     | 0.41              |
| 6:V:339:HIS:CD2   | 6:V:359:ASN:HD21  | 2.38                     | 0.41              |
| 6:V:496:ILE:O     | 6:V:499:ILE:HG13  | 2.20                     | 0.41              |
| 1:B:608:ARG:HA    | 1:B:611:ARG:HG2   | 2.00                     | 0.41              |
| 1:B:1316:LYS:HD3  | 1:B:1316:LYS:HA   | 1.68                     | 0.41              |
| 1:F:174:ILE:HG13  | 1:F:175:GLN:N     | 2.35                     | 0.41              |
| 1:F:1157:MET:HG3  | 1:F:1163:THR:HG21 | 2.03                     | 0.41              |
| 1:F:1182:LEU:HD13 | 1:F:1182:LEU:HA   | 1.96                     | 0.41              |
| 2:K:28:THR:HB     | 2:K:29:PRO:HD3    | 2.02                     | 0.41              |
| 1:L:1361:MET:HG3  | 1:L:1362:LEU:HD12 | 2.01                     | 0.41              |
| 4:O:251:GLN:H     | 4:O:251:GLN:HG2   | 1.64                     | 0.41              |
| 3:Q:198:LEU:HD12  | 3:Q:201:ILE:HD11  | 2.02                     | 0.41              |
| 4:R:117:PRO:HG3   | 4:R:138:LEU:HD13  | 2.02                     | 0.41              |
| 6:U:454:THR:HB    | 6:U:460:PHE:HB3   | 2.03                     | 0.41              |
| 6:U:490:GLN:H     | 6:U:490:GLN:HG3   | 1.65                     | 0.41              |
| 1:B:116:ILE:CA    | 1:D:191:GLY:HA3   | 2.51                     | 0.41              |
| 1:D:940:ALA:H     | 1:D:1157:MET:HE2  | 1.85                     | 0.41              |
| 2:K:26:ALA:C      | 2:K:29:PRO:HD2    | 2.45                     | 0.41              |
| 6:U:136:ILE:HA    | 6:U:142:PRO:HB3   | 2.02                     | 0.41              |
| 1:A:142:SER:HB3   | 1:A:1113:THR:HG22 | 2.01                     | 0.41              |
| 1:D:79:PHE:HD1    | 1:D:79:PHE:HA     | 1.78                     | 0.41              |
| 1:D:841:SER:HB2   | 1:D:844:SER:HB3   | 2.02                     | 0.41              |
| 1:D:1273:ASP:O    | 1:D:1277:ASN:HB2  | 2.21                     | 0.41              |
| 1:F:279:ASN:HD22  | 1:F:384:LEU:HD13  | 1.85                     | 0.41              |
| 1:J:611:ARG:HD3   | 1:J:1063:PHE:HE1  | 1.85                     | 0.41              |
| 4:P:114:LEU:HD22  | 4:P:137:PRO:HG2   | 2.03                     | 0.41              |
| 5:T:354:ARG:HB3   | 5:T:376:ASN:HD22  | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:447:GLN:HG3   | 1:B:617:LEU:HD12  | 2.02                     | 0.41              |
| 1:D:549:ALA:O     | 1:D:550:PRO:C     | 2.63                     | 0.41              |
| 1:F:200:LEU:HD22  | 1:F:203:LYS:HE3   | 2.03                     | 0.41              |
| 1:F:1059:LEU:HA   | 1:F:1063:PHE:HA   | 2.02                     | 0.41              |
| 1:H:545:LEU:HD13  | 1:H:548:ILE:HD11  | 2.01                     | 0.41              |
| 1:J:569:PRO:HG3   | 1:J:585:PRO:HA    | 2.03                     | 0.41              |
| 1:J:592:ARG:HH21  | 1:J:594:ILE:HB    | 1.86                     | 0.41              |
| 1:J:1376:HIS:HD2  | 1:J:1377:LEU:HG   | 1.85                     | 0.41              |
| 1:L:304:LEU:HD12  | 1:L:304:LEU:HA    | 1.81                     | 0.41              |
| 4:S:97:PHE:HE1    | 4:S:310:ARG:HE    | 1.68                     | 0.41              |
| 1:F:384:LEU:HD23  | 1:F:393:PHE:HB3   | 2.03                     | 0.41              |
| 1:L:96:PHE:HB2    | 1:L:99:LEU:HD12   | 2.03                     | 0.41              |
| 3:Q:325:PHE:HB2   | 3:Q:436:ALA:HB3   | 2.02                     | 0.41              |
| 5:T:88:LYS:HE2    | 5:T:90:GLU:HG2    | 2.03                     | 0.41              |
| 1:D:214:ASN:HA    | 1:D:217:GLN:HE21  | 1.86                     | 0.41              |
| 2:G:41:PRO:HB2    | 2:G:44:PRO:HD2    | 2.03                     | 0.41              |
| 1:H:1004:LYS:HD3  | 1:H:1004:LYS:HA   | 1.63                     | 0.41              |
| 1:L:544:ILE:HG23  | 1:L:545:LEU:H     | 1.86                     | 0.41              |
| 3:N:178:ALA:HB2   | 3:N:237:ARG:HH11  | 1.85                     | 0.41              |
| 4:O:223:ILE:HG13  | 4:O:224:PRO:CD    | 2.51                     | 0.41              |
| 1:A:116:ILE:HD12  | 1:A:116:ILE:HA    | 1.92                     | 0.41              |
| 1:A:552:ASN:O     | 1:A:556:ARG:HB3   | 2.21                     | 0.41              |
| 1:B:117:ALA:O     | 1:D:193:ALA:HB3   | 2.21                     | 0.41              |
| 1:B:222:LEU:HB2   | 1:B:226:ALA:HB3   | 2.02                     | 0.41              |
| 1:B:402:TYR:HD1   | 1:B:402:TYR:HA    | 1.79                     | 0.41              |
| 1:B:739:LEU:HD11  | 1:B:1051:THR:HG21 | 2.03                     | 0.41              |
| 1:B:855:LEU:HG    | 2:E:93:ARG:HD2    | 2.03                     | 0.41              |
| 1:D:263:VAL:HG21  | 1:D:390:LYS:HD2   | 2.02                     | 0.41              |
| 1:F:300:LEU:HA    | 1:F:304:LEU:HB2   | 2.03                     | 0.41              |
| 1:F:1215:LEU:HG   | 1:F:1219:ARG:HE   | 1.86                     | 0.41              |
| 1:H:552:ASN:HD21  | 1:H:1249:THR:HG22 | 1.85                     | 0.41              |
| 1:H:1021:ILE:HG21 | 1:H:1025:VAL:HG13 | 2.03                     | 0.41              |
| 1:H:1080:GLU:HB2  | 1:H:1132:ALA:HB1  | 2.01                     | 0.41              |
| 2:K:96:VAL:HG11   | 1:L:894:LEU:HB3   | 2.03                     | 0.41              |
| 1:L:203:LYS:HD2   | 1:L:203:LYS:HA    | 1.59                     | 0.41              |
| 1:L:758:ALA:HB1   | 1:L:830:LYS:HZ1   | 1.85                     | 0.41              |
| 3:Q:345:LEU:HD12  | 3:Q:345:LEU:HA    | 1.88                     | 0.41              |
| 7:X:12:CYS:O      | 7:X:15:MET:HG2    | 2.21                     | 0.41              |
| 1:D:250:ARG:HG3   | 1:D:251:GLU:HG2   | 2.02                     | 0.41              |
| 1:H:639:TYR:HB2   | 1:H:959:MET:HB3   | 2.03                     | 0.41              |
| 1:H:1026:ALA:HA   | 1:H:1029:VAL:HG12 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:600:VAL:HB   | 1:J:601:PRO:HD3   | 2.02                     | 0.41              |
| 1:L:1245:MET:HE2 | 1:L:1245:MET:HB2  | 1.91                     | 0.41              |
| 3:Q:168:LEU:HD23 | 3:Q:168:LEU:HA    | 1.95                     | 0.41              |
| 1:A:674:GLN:HG3  | 1:A:675:SER:N     | 2.36                     | 0.40              |
| 1:B:99:LEU:HD12  | 1:B:99:LEU:HA     | 1.93                     | 0.40              |
| 1:D:242:MET:HG3  | 1:D:243:PHE:H     | 1.85                     | 0.40              |
| 1:J:1176:LEU:HA  | 1:L:1247:ASP:HB3  | 2.03                     | 0.40              |
| 1:L:54:ILE:HG12  | 1:L:58:ASP:HB2    | 2.02                     | 0.40              |
| 5:T:598:LYS:HB2  | 5:T:598:LYS:HE3   | 1.85                     | 0.40              |
| 1:A:995:MET:HG3  | 1:A:1000:ARG:HG3  | 2.03                     | 0.40              |
| 1:F:138:LYS:HE2  | 1:F:138:LYS:HB3   | 1.90                     | 0.40              |
| 1:F:295:LEU:HD23 | 1:F:295:LEU:HA    | 1.94                     | 0.40              |
| 1:F:399:ARG:HD2  | 1:F:399:ARG:HA    | 1.84                     | 0.40              |
| 1:F:794:PHE:HZ   | 1:F:852:TYR:HB2   | 1.87                     | 0.40              |
| 1:F:834:TYR:HD1  | 1:F:834:TYR:HA    | 1.76                     | 0.40              |
| 1:J:660:LEU:HD23 | 1:J:660:LEU:HA    | 1.86                     | 0.40              |
| 1:L:386:ILE:HG23 | 1:L:391:LEU:HG    | 2.03                     | 0.40              |
| 6:U:266:GLU:HA   | 6:U:269:VAL:HG22  | 2.03                     | 0.40              |
| 6:U:491:TYR:HD1  | 6:U:491:TYR:HA    | 1.78                     | 0.40              |
| 6:V:499:ILE:O    | 6:V:502:GLU:HG3   | 2.20                     | 0.40              |
| 6:V:539:GLN:H    | 6:V:539:GLN:HG3   | 1.66                     | 0.40              |
| 1:B:488:ALA:HB3  | 1:B:1274:ARG:NH2  | 2.36                     | 0.40              |
| 1:F:103:ARG:HH12 | 1:F:335:LYS:HA    | 1.86                     | 0.40              |
| 1:F:108:GLN:H    | 1:F:108:GLN:HG3   | 1.73                     | 0.40              |
| 1:F:548:ILE:HD13 | 1:F:1258:ARG:HE   | 1.86                     | 0.40              |
| 1:F:938:ALA:HB2  | 1:F:1158:LEU:HD22 | 2.04                     | 0.40              |
| 1:J:171:ILE:HD13 | 1:J:171:ILE:HA    | 1.94                     | 0.40              |
| 1:J:766:ALA:HA   | 1:J:769:ARG:HE    | 1.86                     | 0.40              |
| 1:L:622:MET:HE3  | 1:L:713:HIS:CE1   | 2.56                     | 0.40              |
| 6:U:87:PRO:O     | 6:U:90:GLU:HG3    | 2.21                     | 0.40              |
| 6:U:539:GLN:HB3  | 6:U:541:ARG:HH21  | 1.85                     | 0.40              |
| 1:A:304:LEU:HD22 | 1:A:385:VAL:HG21  | 2.04                     | 0.40              |
| 1:A:1166:LEU:HA  | 1:A:1169:ILE:HG12 | 2.03                     | 0.40              |
| 1:H:237:ARG:O    | 1:H:241:ASP:HB2   | 2.21                     | 0.40              |
| 1:H:243:PHE:HE2  | 1:H:1388:LEU:HB2  | 1.86                     | 0.40              |
| 1:H:830:LYS:O    | 1:H:834:TYR:HB2   | 2.21                     | 0.40              |
| 1:H:862:VAL:HG22 | 1:H:913:LEU:HD21  | 2.03                     | 0.40              |
| 1:J:945:MET:H    | 1:J:945:MET:HG3   | 1.62                     | 0.40              |
| 1:L:1019:ALA:HB3 | 1:L:1021:ILE:HD11 | 2.03                     | 0.40              |
| 2:M:56:ILE:HA    | 2:M:59:VAL:HG22   | 2.02                     | 0.40              |
| 3:N:212:LYS:H    | 3:N:212:LYS:HG3   | 1.60                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:P:302:PRO:HG3  | 4:P:311:THR:HG23 | 2.04                     | 0.40              |
| 5:T:359:VAL:HB   | 5:T:372:VAL:HB   | 2.04                     | 0.40              |
| 5:T:431:ASN:HA   | 5:T:434:ASN:HD21 | 1.86                     | 0.40              |
| 6:U:321:PRO:HA   | 6:U:322:PRO:HD3  | 1.98                     | 0.40              |
| 6:V:356:ARG:HD2  | 6:V:356:ARG:HA   | 1.84                     | 0.40              |
| 7:W:12:CYS:O     | 7:W:15:MET:HG2   | 2.21                     | 0.40              |
| 1:A:880:PRO:HA   | 1:A:887:HIS:HB3  | 2.03                     | 0.40              |
| 1:B:259:LEU:HD13 | 1:B:388:GLY:HA2  | 2.02                     | 0.40              |
| 1:F:1231:MET:H   | 1:F:1231:MET:HG3 | 1.69                     | 0.40              |
| 1:L:104:ASP:HB3  | 1:L:105:GLY:H    | 1.67                     | 0.40              |
| 1:L:178:ALA:O    | 1:L:181:LEU:HG   | 2.21                     | 0.40              |
| 1:L:846:CYS:HB2  | 1:L:985:CYS:HB3  | 1.82                     | 0.40              |
| 5:T:422:LEU:HD12 | 5:T:422:LEU:HA   | 1.94                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | A     | 1148/1396 (82%) | 1081 (94%) | 63 (6%) | 4 (0%)   | 36          | 72  |
| 1   | B     | 1324/1396 (95%) | 1252 (95%) | 70 (5%) | 2 (0%)   | 43          | 78  |
| 1   | D     | 1331/1396 (95%) | 1238 (93%) | 87 (6%) | 6 (0%)   | 24          | 63  |
| 1   | F     | 1331/1396 (95%) | 1268 (95%) | 58 (4%) | 5 (0%)   | 30          | 67  |
| 1   | H     | 1271/1396 (91%) | 1213 (95%) | 55 (4%) | 3 (0%)   | 43          | 78  |
| 1   | J     | 1269/1396 (91%) | 1189 (94%) | 76 (6%) | 4 (0%)   | 36          | 72  |
| 1   | L     | 1308/1396 (94%) | 1231 (94%) | 72 (6%) | 5 (0%)   | 30          | 67  |
| 2   | C     | 99/235 (42%)    | 93 (94%)   | 5 (5%)  | 1 (1%)   | 12          | 49  |
| 2   | E     | 93/235 (40%)    | 90 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 2   | G     | 99/235 (42%)    | 93 (94%)   | 6 (6%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 2   | I     | 99/235 (42%)      | 95 (96%)    | 4 (4%)   | 0        | 100         | 100 |
| 2   | K     | 99/235 (42%)      | 94 (95%)    | 5 (5%)   | 0        | 100         | 100 |
| 2   | M     | 99/235 (42%)      | 90 (91%)    | 9 (9%)   | 0        | 100         | 100 |
| 3   | N     | 353/483 (73%)     | 337 (96%)   | 16 (4%)  | 0        | 100         | 100 |
| 3   | Q     | 353/483 (73%)     | 341 (97%)   | 12 (3%)  | 0        | 100         | 100 |
| 4   | O     | 294/316 (93%)     | 283 (96%)   | 9 (3%)   | 2 (1%)   | 18          | 56  |
| 4   | P     | 271/316 (86%)     | 261 (96%)   | 9 (3%)   | 1 (0%)   | 30          | 67  |
| 4   | R     | 294/316 (93%)     | 283 (96%)   | 9 (3%)   | 2 (1%)   | 18          | 56  |
| 4   | S     | 271/316 (86%)     | 263 (97%)   | 8 (3%)   | 0        | 100         | 100 |
| 5   | T     | 589/676 (87%)     | 558 (95%)   | 29 (5%)  | 2 (0%)   | 36          | 72  |
| 6   | U     | 529/579 (91%)     | 466 (88%)   | 55 (10%) | 8 (2%)   | 8           | 40  |
| 6   | V     | 529/579 (91%)     | 464 (88%)   | 60 (11%) | 5 (1%)   | 14          | 51  |
| 7   | W     | 43/2763 (2%)      | 43 (100%)   | 0        | 0        | 100         | 100 |
| 7   | X     | 43/2763 (2%)      | 43 (100%)   | 0        | 0        | 100         | 100 |
| All | All   | 13139/20772 (63%) | 12369 (94%) | 720 (6%) | 50 (0%)  | 31          | 67  |

All (50) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 392  | VAL  |
| 1   | A     | 425  | VAL  |
| 1   | D     | 550  | PRO  |
| 1   | D     | 1241 | ILE  |
| 1   | F     | 599  | PRO  |
| 1   | H     | 550  | PRO  |
| 1   | L     | 68   | ILE  |
| 1   | L     | 640  | PRO  |
| 5   | T     | 207  | VAL  |
| 6   | U     | 130  | ILE  |
| 6   | U     | 168  | PRO  |
| 6   | U     | 248  | GLU  |
| 6   | U     | 417  | VAL  |
| 6   | V     | 391  | VAL  |
| 1   | A     | 506  | VAL  |
| 1   | F     | 1023 | GLN  |
| 1   | H     | 593  | ILE  |
| 1   | J     | 1180 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | O     | 43   | VAL  |
| 4   | O     | 52   | ILE  |
| 6   | U     | 194  | VAL  |
| 6   | U     | 418  | ILE  |
| 6   | U     | 510  | VAL  |
| 6   | V     | 510  | VAL  |
| 2   | C     | 15   | ASN  |
| 1   | L     | 552  | ASN  |
| 4   | R     | 16   | SER  |
| 5   | T     | 482  | TYR  |
| 1   | D     | 440  | ASP  |
| 6   | V     | 322  | PRO  |
| 6   | V     | 360  | VAL  |
| 1   | B     | 436  | ARG  |
| 1   | D     | 508  | VAL  |
| 1   | F     | 1392 | LEU  |
| 1   | J     | 890  | VAL  |
| 1   | L     | 508  | VAL  |
| 6   | U     | 136  | ILE  |
| 6   | V     | 246  | VAL  |
| 1   | A     | 1096 | GLN  |
| 1   | F     | 37   | SER  |
| 1   | J     | 508  | VAL  |
| 1   | J     | 1364 | THR  |
| 1   | B     | 508  | VAL  |
| 1   | H     | 508  | VAL  |
| 1   | D     | 601  | PRO  |
| 4   | P     | 166  | ILE  |
| 4   | R     | 52   | ILE  |
| 1   | D     | 890  | VAL  |
| 1   | L     | 890  | VAL  |
| 1   | F     | 639  | TYR  |

### 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     | 964/1182 (82%)    | 918 (95%)   | 46 (5%)  | 23          | 44  |
| 1   | B     | 1097/1182 (93%)   | 1044 (95%)  | 53 (5%)  | 23          | 44  |
| 1   | D     | 1087/1182 (92%)   | 1043 (96%)  | 44 (4%)  | 28          | 49  |
| 1   | F     | 1102/1182 (93%)   | 1066 (97%)  | 36 (3%)  | 33          | 55  |
| 1   | H     | 1040/1182 (88%)   | 1001 (96%)  | 39 (4%)  | 29          | 50  |
| 1   | J     | 1050/1182 (89%)   | 1009 (96%)  | 41 (4%)  | 28          | 49  |
| 1   | L     | 1089/1182 (92%)   | 1048 (96%)  | 41 (4%)  | 29          | 50  |
| 2   | C     | 72/189 (38%)      | 71 (99%)    | 1 (1%)   | 59          | 72  |
| 2   | E     | 72/189 (38%)      | 67 (93%)    | 5 (7%)   | 14          | 36  |
| 2   | G     | 74/189 (39%)      | 73 (99%)    | 1 (1%)   | 59          | 72  |
| 2   | I     | 75/189 (40%)      | 74 (99%)    | 1 (1%)   | 61          | 74  |
| 2   | K     | 75/189 (40%)      | 71 (95%)    | 4 (5%)   | 20          | 41  |
| 2   | M     | 71/189 (38%)      | 71 (100%)   | 0        | 100         | 100 |
| 3   | N     | 288/410 (70%)     | 282 (98%)   | 6 (2%)   | 47          | 65  |
| 3   | Q     | 289/410 (70%)     | 281 (97%)   | 8 (3%)   | 38          | 60  |
| 4   | O     | 256/267 (96%)     | 247 (96%)   | 9 (4%)   | 32          | 53  |
| 4   | P     | 229/267 (86%)     | 224 (98%)   | 5 (2%)   | 45          | 64  |
| 4   | R     | 256/267 (96%)     | 247 (96%)   | 9 (4%)   | 32          | 53  |
| 4   | S     | 230/267 (86%)     | 217 (94%)   | 13 (6%)  | 18          | 40  |
| 5   | T     | 503/573 (88%)     | 487 (97%)   | 16 (3%)  | 34          | 56  |
| 6   | U     | 457/497 (92%)     | 440 (96%)   | 17 (4%)  | 30          | 51  |
| 6   | V     | 457/497 (92%)     | 431 (94%)   | 26 (6%)  | 18          | 40  |
| 7   | W     | 38/2413 (2%)      | 37 (97%)    | 1 (3%)   | 40          | 62  |
| 7   | X     | 38/2413 (2%)      | 37 (97%)    | 1 (3%)   | 40          | 62  |
| All | All   | 10909/17689 (62%) | 10486 (96%) | 423 (4%) | 30          | 49  |

All (423) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 102 | VAL  |
| 1   | A     | 133 | VAL  |
| 1   | A     | 189 | GLU  |
| 1   | A     | 225 | VAL  |
| 1   | A     | 254 | LEU  |
| 1   | A     | 300 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 313  | VAL  |
| 1   | A     | 393  | PHE  |
| 1   | A     | 425  | VAL  |
| 1   | A     | 466  | LEU  |
| 1   | A     | 486  | VAL  |
| 1   | A     | 542  | LEU  |
| 1   | A     | 543  | THR  |
| 1   | A     | 591  | LEU  |
| 1   | A     | 600  | VAL  |
| 1   | A     | 623  | THR  |
| 1   | A     | 632  | ASP  |
| 1   | A     | 643  | PHE  |
| 1   | A     | 644  | TYR  |
| 1   | A     | 673  | GLU  |
| 1   | A     | 681  | VAL  |
| 1   | A     | 706  | ILE  |
| 1   | A     | 710  | LEU  |
| 1   | A     | 721  | ILE  |
| 1   | A     | 764  | GLU  |
| 1   | A     | 834  | TYR  |
| 1   | A     | 852  | TYR  |
| 1   | A     | 856  | TYR  |
| 1   | A     | 867  | ILE  |
| 1   | A     | 875  | THR  |
| 1   | A     | 890  | VAL  |
| 1   | A     | 903  | LEU  |
| 1   | A     | 905  | VAL  |
| 1   | A     | 954  | HIS  |
| 1   | A     | 977  | VAL  |
| 1   | A     | 1006 | VAL  |
| 1   | A     | 1029 | VAL  |
| 1   | A     | 1099 | VAL  |
| 1   | A     | 1114 | GLN  |
| 1   | A     | 1146 | GLN  |
| 1   | A     | 1164 | GLU  |
| 1   | A     | 1172 | SER  |
| 1   | A     | 1313 | MET  |
| 1   | A     | 1340 | THR  |
| 1   | A     | 1346 | LEU  |
| 1   | A     | 1388 | LEU  |
| 1   | B     | 25   | ILE  |
| 1   | B     | 61   | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 68   | ILE  |
| 1   | B     | 78   | ASN  |
| 1   | B     | 85   | LEU  |
| 1   | B     | 89   | VAL  |
| 1   | B     | 106  | VAL  |
| 1   | B     | 116  | ILE  |
| 1   | B     | 169  | LEU  |
| 1   | B     | 189  | GLU  |
| 1   | B     | 222  | LEU  |
| 1   | B     | 234  | LEU  |
| 1   | B     | 270  | VAL  |
| 1   | B     | 285  | VAL  |
| 1   | B     | 306  | ILE  |
| 1   | B     | 387  | VAL  |
| 1   | B     | 411  | LEU  |
| 1   | B     | 435  | THR  |
| 1   | B     | 497  | HIS  |
| 1   | B     | 547  | PHE  |
| 1   | B     | 621  | THR  |
| 1   | B     | 642  | ILE  |
| 1   | B     | 646  | LEU  |
| 1   | B     | 663  | LEU  |
| 1   | B     | 686  | MET  |
| 1   | B     | 702  | VAL  |
| 1   | B     | 719  | GLN  |
| 1   | B     | 726  | ILE  |
| 1   | B     | 739  | LEU  |
| 1   | B     | 743  | LEU  |
| 1   | B     | 815  | ILE  |
| 1   | B     | 859  | LEU  |
| 1   | B     | 862  | VAL  |
| 1   | B     | 890  | VAL  |
| 1   | B     | 896  | VAL  |
| 1   | B     | 905  | VAL  |
| 1   | B     | 914  | GLN  |
| 1   | B     | 922  | GLU  |
| 1   | B     | 964  | TYR  |
| 1   | B     | 977  | VAL  |
| 1   | B     | 1029 | VAL  |
| 1   | B     | 1047 | TYR  |
| 1   | B     | 1059 | LEU  |
| 1   | B     | 1072 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1155 | VAL  |
| 1   | B     | 1222 | CYS  |
| 1   | B     | 1288 | ILE  |
| 1   | B     | 1289 | TYR  |
| 1   | B     | 1293 | PHE  |
| 1   | B     | 1297 | THR  |
| 1   | B     | 1308 | LEU  |
| 1   | B     | 1337 | THR  |
| 1   | B     | 1374 | GLU  |
| 2   | C     | 42   | LEU  |
| 1   | D     | 111  | VAL  |
| 1   | D     | 165  | ILE  |
| 1   | D     | 197  | LEU  |
| 1   | D     | 223  | ASN  |
| 1   | D     | 272  | VAL  |
| 1   | D     | 315  | VAL  |
| 1   | D     | 322  | LEU  |
| 1   | D     | 405  | THR  |
| 1   | D     | 435  | THR  |
| 1   | D     | 444  | VAL  |
| 1   | D     | 495  | GLN  |
| 1   | D     | 496  | GLN  |
| 1   | D     | 529  | ASP  |
| 1   | D     | 543  | THR  |
| 1   | D     | 544  | ILE  |
| 1   | D     | 567  | VAL  |
| 1   | D     | 574  | LEU  |
| 1   | D     | 623  | THR  |
| 1   | D     | 651  | HIS  |
| 1   | D     | 667  | CYS  |
| 1   | D     | 702  | VAL  |
| 1   | D     | 752  | ILE  |
| 1   | D     | 753  | LEU  |
| 1   | D     | 775  | VAL  |
| 1   | D     | 818  | THR  |
| 1   | D     | 853  | ASP  |
| 1   | D     | 864  | VAL  |
| 1   | D     | 867  | ILE  |
| 1   | D     | 890  | VAL  |
| 1   | D     | 896  | VAL  |
| 1   | D     | 941  | THR  |
| 1   | D     | 947  | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 958  | MET  |
| 1   | D     | 1005 | MET  |
| 1   | D     | 1006 | VAL  |
| 1   | D     | 1071 | VAL  |
| 1   | D     | 1148 | LEU  |
| 1   | D     | 1232 | LEU  |
| 1   | D     | 1279 | THR  |
| 1   | D     | 1282 | LEU  |
| 1   | D     | 1303 | THR  |
| 1   | D     | 1306 | ASN  |
| 1   | D     | 1324 | THR  |
| 1   | D     | 1364 | THR  |
| 2   | E     | 90   | THR  |
| 2   | E     | 95   | THR  |
| 2   | E     | 96   | VAL  |
| 2   | E     | 98   | LEU  |
| 2   | E     | 100  | ARG  |
| 1   | F     | 37   | SER  |
| 1   | F     | 48   | PHE  |
| 1   | F     | 80   | VAL  |
| 1   | F     | 84   | GLU  |
| 1   | F     | 85   | LEU  |
| 1   | F     | 102  | VAL  |
| 1   | F     | 158  | THR  |
| 1   | F     | 301  | GLN  |
| 1   | F     | 309  | THR  |
| 1   | F     | 329  | THR  |
| 1   | F     | 380  | VAL  |
| 1   | F     | 444  | VAL  |
| 1   | F     | 473  | ASP  |
| 1   | F     | 493  | LEU  |
| 1   | F     | 543  | THR  |
| 1   | F     | 544  | ILE  |
| 1   | F     | 555  | LEU  |
| 1   | F     | 602  | LEU  |
| 1   | F     | 770  | LEU  |
| 1   | F     | 818  | THR  |
| 1   | F     | 834  | TYR  |
| 1   | F     | 859  | LEU  |
| 1   | F     | 864  | VAL  |
| 1   | F     | 867  | ILE  |
| 1   | F     | 903  | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 916  | LEU  |
| 1   | F     | 967  | THR  |
| 1   | F     | 977  | VAL  |
| 1   | F     | 979  | VAL  |
| 1   | F     | 1051 | THR  |
| 1   | F     | 1128 | VAL  |
| 1   | F     | 1182 | LEU  |
| 1   | F     | 1188 | LEU  |
| 1   | F     | 1279 | THR  |
| 1   | F     | 1318 | VAL  |
| 1   | F     | 1327 | GLU  |
| 2   | G     | 17   | THR  |
| 1   | H     | 77   | LEU  |
| 1   | H     | 89   | VAL  |
| 1   | H     | 92   | ILE  |
| 1   | H     | 111  | VAL  |
| 1   | H     | 141  | LEU  |
| 1   | H     | 215  | LYS  |
| 1   | H     | 235  | LYS  |
| 1   | H     | 272  | VAL  |
| 1   | H     | 290  | VAL  |
| 1   | H     | 320  | MET  |
| 1   | H     | 327  | LEU  |
| 1   | H     | 328  | VAL  |
| 1   | H     | 331  | LEU  |
| 1   | H     | 380  | VAL  |
| 1   | H     | 385  | VAL  |
| 1   | H     | 444  | VAL  |
| 1   | H     | 457  | ILE  |
| 1   | H     | 497  | HIS  |
| 1   | H     | 542  | LEU  |
| 1   | H     | 607  | PHE  |
| 1   | H     | 623  | THR  |
| 1   | H     | 646  | LEU  |
| 1   | H     | 742  | ILE  |
| 1   | H     | 757  | ASP  |
| 1   | H     | 759  | LEU  |
| 1   | H     | 764  | GLU  |
| 1   | H     | 775  | VAL  |
| 1   | H     | 818  | THR  |
| 1   | H     | 834  | TYR  |
| 1   | H     | 864  | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | H     | 876  | THR  |
| 1   | H     | 1121 | LEU  |
| 1   | H     | 1158 | LEU  |
| 1   | H     | 1182 | LEU  |
| 1   | H     | 1192 | THR  |
| 1   | H     | 1217 | TYR  |
| 1   | H     | 1256 | THR  |
| 1   | H     | 1301 | VAL  |
| 1   | H     | 1346 | LEU  |
| 2   | I     | 17   | THR  |
| 1   | J     | 242  | MET  |
| 1   | J     | 270  | VAL  |
| 1   | J     | 327  | LEU  |
| 1   | J     | 380  | VAL  |
| 1   | J     | 457  | ILE  |
| 1   | J     | 475  | MET  |
| 1   | J     | 490  | LEU  |
| 1   | J     | 531  | MET  |
| 1   | J     | 538  | VAL  |
| 1   | J     | 544  | ILE  |
| 1   | J     | 567  | VAL  |
| 1   | J     | 613  | THR  |
| 1   | J     | 673  | GLU  |
| 1   | J     | 693  | TYR  |
| 1   | J     | 713  | HIS  |
| 1   | J     | 724  | PHE  |
| 1   | J     | 764  | GLU  |
| 1   | J     | 815  | ILE  |
| 1   | J     | 835  | ILE  |
| 1   | J     | 850  | VAL  |
| 1   | J     | 855  | LEU  |
| 1   | J     | 890  | VAL  |
| 1   | J     | 905  | VAL  |
| 1   | J     | 916  | LEU  |
| 1   | J     | 939  | THR  |
| 1   | J     | 947  | ILE  |
| 1   | J     | 1006 | VAL  |
| 1   | J     | 1009 | ILE  |
| 1   | J     | 1027 | TYR  |
| 1   | J     | 1071 | VAL  |
| 1   | J     | 1111 | THR  |
| 1   | J     | 1121 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | J     | 1126 | THR  |
| 1   | J     | 1162 | VAL  |
| 1   | J     | 1166 | LEU  |
| 1   | J     | 1188 | LEU  |
| 1   | J     | 1242 | GLU  |
| 1   | J     | 1245 | MET  |
| 1   | J     | 1271 | TYR  |
| 1   | J     | 1375 | VAL  |
| 1   | J     | 1381 | LEU  |
| 2   | K     | 36   | LEU  |
| 2   | K     | 42   | LEU  |
| 2   | K     | 80   | THR  |
| 2   | K     | 98   | LEU  |
| 1   | L     | 36   | LEU  |
| 1   | L     | 68   | ILE  |
| 1   | L     | 106  | VAL  |
| 1   | L     | 124  | VAL  |
| 1   | L     | 158  | THR  |
| 1   | L     | 203  | LYS  |
| 1   | L     | 207  | LEU  |
| 1   | L     | 221  | HIS  |
| 1   | L     | 222  | LEU  |
| 1   | L     | 231  | LEU  |
| 1   | L     | 313  | VAL  |
| 1   | L     | 394  | LEU  |
| 1   | L     | 415  | ILE  |
| 1   | L     | 420  | ILE  |
| 1   | L     | 503  | TYR  |
| 1   | L     | 506  | VAL  |
| 1   | L     | 544  | ILE  |
| 1   | L     | 545  | LEU  |
| 1   | L     | 602  | LEU  |
| 1   | L     | 622  | MET  |
| 1   | L     | 623  | THR  |
| 1   | L     | 703  | CYS  |
| 1   | L     | 722  | THR  |
| 1   | L     | 741  | ASN  |
| 1   | L     | 784  | LEU  |
| 1   | L     | 787  | VAL  |
| 1   | L     | 801  | LEU  |
| 1   | L     | 828  | LEU  |
| 1   | L     | 834  | TYR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L     | 864  | VAL  |
| 1   | L     | 1006 | VAL  |
| 1   | L     | 1050 | PHE  |
| 1   | L     | 1059 | LEU  |
| 1   | L     | 1072 | VAL  |
| 1   | L     | 1131 | THR  |
| 1   | L     | 1148 | LEU  |
| 1   | L     | 1155 | VAL  |
| 1   | L     | 1182 | LEU  |
| 1   | L     | 1203 | VAL  |
| 1   | L     | 1290 | SER  |
| 1   | L     | 1379 | GLN  |
| 3   | N     | 159  | THR  |
| 3   | N     | 240  | GLU  |
| 3   | N     | 313  | LEU  |
| 3   | N     | 401  | ILE  |
| 3   | N     | 404  | ILE  |
| 3   | N     | 407  | VAL  |
| 4   | O     | 19   | GLU  |
| 4   | O     | 64   | GLU  |
| 4   | O     | 78   | ILE  |
| 4   | O     | 132  | LEU  |
| 4   | O     | 140  | ILE  |
| 4   | O     | 144  | LEU  |
| 4   | O     | 223  | ILE  |
| 4   | O     | 238  | LEU  |
| 4   | O     | 314  | ILE  |
| 4   | P     | 8    | GLU  |
| 4   | P     | 14   | GLU  |
| 4   | P     | 47   | LEU  |
| 4   | P     | 63   | LEU  |
| 4   | P     | 143  | THR  |
| 3   | Q     | 167  | VAL  |
| 3   | Q     | 195  | VAL  |
| 3   | Q     | 236  | ILE  |
| 3   | Q     | 242  | LEU  |
| 3   | Q     | 267  | ILE  |
| 3   | Q     | 313  | LEU  |
| 3   | Q     | 323  | LEU  |
| 3   | Q     | 324  | VAL  |
| 4   | R     | 16   | SER  |
| 4   | R     | 45   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | R     | 115 | LEU  |
| 4   | R     | 160 | THR  |
| 4   | R     | 177 | VAL  |
| 4   | R     | 216 | CYS  |
| 4   | R     | 255 | ILE  |
| 4   | R     | 283 | ARG  |
| 4   | R     | 296 | VAL  |
| 4   | S     | 10  | LEU  |
| 4   | S     | 35  | THR  |
| 4   | S     | 60  | LEU  |
| 4   | S     | 75  | THR  |
| 4   | S     | 91  | THR  |
| 4   | S     | 112 | ILE  |
| 4   | S     | 125 | ILE  |
| 4   | S     | 140 | ILE  |
| 4   | S     | 167 | LEU  |
| 4   | S     | 204 | LEU  |
| 4   | S     | 210 | PHE  |
| 4   | S     | 218 | LEU  |
| 4   | S     | 220 | LEU  |
| 5   | T     | 22  | LEU  |
| 5   | T     | 23  | LEU  |
| 5   | T     | 84  | LEU  |
| 5   | T     | 90  | GLU  |
| 5   | T     | 159 | GLN  |
| 5   | T     | 168 | LEU  |
| 5   | T     | 175 | THR  |
| 5   | T     | 185 | TYR  |
| 5   | T     | 241 | LEU  |
| 5   | T     | 439 | LEU  |
| 5   | T     | 469 | GLU  |
| 5   | T     | 482 | TYR  |
| 5   | T     | 499 | THR  |
| 5   | T     | 509 | VAL  |
| 5   | T     | 580 | VAL  |
| 5   | T     | 651 | LEU  |
| 6   | U     | 51  | LEU  |
| 6   | U     | 111 | GLU  |
| 6   | U     | 123 | GLU  |
| 6   | U     | 130 | ILE  |
| 6   | U     | 146 | ASP  |
| 6   | U     | 235 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | U     | 237 | TYR  |
| 6   | U     | 278 | LYS  |
| 6   | U     | 310 | VAL  |
| 6   | U     | 354 | LEU  |
| 6   | U     | 358 | GLN  |
| 6   | U     | 386 | LEU  |
| 6   | U     | 417 | VAL  |
| 6   | U     | 485 | ASP  |
| 6   | U     | 518 | VAL  |
| 6   | U     | 542 | VAL  |
| 6   | U     | 565 | TYR  |
| 6   | V     | 79  | THR  |
| 6   | V     | 110 | GLU  |
| 6   | V     | 145 | TYR  |
| 6   | V     | 151 | VAL  |
| 6   | V     | 157 | VAL  |
| 6   | V     | 259 | GLU  |
| 6   | V     | 260 | HIS  |
| 6   | V     | 273 | THR  |
| 6   | V     | 288 | LEU  |
| 6   | V     | 319 | VAL  |
| 6   | V     | 320 | LEU  |
| 6   | V     | 354 | LEU  |
| 6   | V     | 355 | GLU  |
| 6   | V     | 387 | TRP  |
| 6   | V     | 391 | VAL  |
| 6   | V     | 402 | LEU  |
| 6   | V     | 450 | LEU  |
| 6   | V     | 483 | VAL  |
| 6   | V     | 502 | GLU  |
| 6   | V     | 511 | THR  |
| 6   | V     | 529 | TYR  |
| 6   | V     | 538 | HIS  |
| 6   | V     | 539 | GLN  |
| 6   | V     | 561 | TYR  |
| 6   | V     | 564 | LEU  |
| 6   | V     | 578 | THR  |
| 7   | W     | 5   | LEU  |
| 7   | X     | 5   | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (219) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 403  | GLN  |
| 1   | A     | 429  | ASN  |
| 1   | A     | 495  | GLN  |
| 1   | A     | 519  | GLN  |
| 1   | A     | 533  | HIS  |
| 1   | A     | 536  | HIS  |
| 1   | A     | 546  | GLN  |
| 1   | A     | 552  | ASN  |
| 1   | A     | 595  | ASN  |
| 1   | A     | 799  | ASN  |
| 1   | A     | 899  | HIS  |
| 1   | A     | 1057 | HIS  |
| 1   | A     | 1058 | GLN  |
| 1   | A     | 1118 | HIS  |
| 1   | A     | 1267 | GLN  |
| 1   | A     | 1269 | HIS  |
| 1   | B     | 122  | HIS  |
| 1   | B     | 129  | HIS  |
| 1   | B     | 180  | ASN  |
| 1   | B     | 214  | ASN  |
| 1   | B     | 217  | GLN  |
| 1   | B     | 427  | GLN  |
| 1   | B     | 468  | GLN  |
| 1   | B     | 560  | ASN  |
| 1   | B     | 620  | HIS  |
| 1   | B     | 666  | GLN  |
| 1   | B     | 727  | GLN  |
| 1   | B     | 731  | HIS  |
| 1   | B     | 732  | ASN  |
| 1   | B     | 740  | ASN  |
| 1   | B     | 782  | GLN  |
| 1   | B     | 792  | HIS  |
| 1   | B     | 820  | HIS  |
| 1   | B     | 821  | HIS  |
| 1   | B     | 1057 | HIS  |
| 1   | B     | 1058 | GLN  |
| 1   | B     | 1074 | GLN  |
| 1   | B     | 1143 | ASN  |
| 1   | B     | 1147 | ASN  |
| 1   | B     | 1223 | ASN  |
| 1   | B     | 1277 | ASN  |
| 1   | B     | 1302 | ASN  |
| 1   | B     | 1348 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1376 | HIS  |
| 1   | D     | 53   | GLN  |
| 1   | D     | 108  | GLN  |
| 1   | D     | 122  | HIS  |
| 1   | D     | 176  | GLN  |
| 1   | D     | 195  | GLN  |
| 1   | D     | 217  | GLN  |
| 1   | D     | 495  | GLN  |
| 1   | D     | 497  | HIS  |
| 1   | D     | 793  | ASN  |
| 1   | D     | 795  | GLN  |
| 1   | D     | 885  | HIS  |
| 1   | D     | 895  | ASN  |
| 1   | D     | 899  | HIS  |
| 1   | D     | 900  | ASN  |
| 1   | D     | 954  | HIS  |
| 1   | D     | 988  | HIS  |
| 1   | D     | 1058 | GLN  |
| 1   | D     | 1101 | HIS  |
| 1   | D     | 1114 | GLN  |
| 1   | D     | 1118 | HIS  |
| 1   | D     | 1177 | ASN  |
| 1   | D     | 1269 | HIS  |
| 1   | D     | 1304 | ASN  |
| 1   | F     | 65   | GLN  |
| 1   | F     | 112  | GLN  |
| 1   | F     | 126  | GLN  |
| 1   | F     | 129  | HIS  |
| 1   | F     | 267  | GLN  |
| 1   | F     | 277  | HIS  |
| 1   | F     | 284  | GLN  |
| 1   | F     | 429  | ASN  |
| 1   | F     | 447  | GLN  |
| 1   | F     | 468  | GLN  |
| 1   | F     | 656  | ASN  |
| 1   | F     | 713  | HIS  |
| 1   | F     | 740  | ASN  |
| 1   | F     | 882  | HIS  |
| 1   | F     | 895  | ASN  |
| 1   | F     | 1058 | GLN  |
| 1   | F     | 1118 | HIS  |
| 1   | F     | 1143 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 1159 | HIS  |
| 1   | F     | 1262 | ASN  |
| 1   | F     | 1306 | ASN  |
| 1   | F     | 1341 | GLN  |
| 1   | H     | 75   | ASN  |
| 1   | H     | 157  | ASN  |
| 1   | H     | 175  | GLN  |
| 1   | H     | 427  | GLN  |
| 1   | H     | 437  | HIS  |
| 1   | H     | 468  | GLN  |
| 1   | H     | 533  | HIS  |
| 1   | H     | 539  | ASN  |
| 1   | H     | 552  | ASN  |
| 1   | H     | 560  | ASN  |
| 1   | H     | 614  | GLN  |
| 1   | H     | 651  | HIS  |
| 1   | H     | 685  | HIS  |
| 1   | H     | 696  | ASN  |
| 1   | H     | 727  | GLN  |
| 1   | H     | 741  | ASN  |
| 1   | H     | 793  | ASN  |
| 1   | H     | 944  | ASN  |
| 1   | H     | 1017 | HIS  |
| 1   | H     | 1031 | HIS  |
| 1   | H     | 1102 | HIS  |
| 1   | H     | 1304 | ASN  |
| 2   | I     | 15   | ASN  |
| 2   | I     | 72   | HIS  |
| 1   | J     | 122  | HIS  |
| 1   | J     | 137  | HIS  |
| 1   | J     | 468  | GLN  |
| 1   | J     | 533  | HIS  |
| 1   | J     | 546  | GLN  |
| 1   | J     | 597  | ASN  |
| 1   | J     | 653  | ASN  |
| 1   | J     | 656  | ASN  |
| 1   | J     | 713  | HIS  |
| 1   | J     | 727  | GLN  |
| 1   | J     | 741  | ASN  |
| 1   | J     | 860  | GLN  |
| 1   | J     | 885  | HIS  |
| 1   | J     | 887  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | J     | 914  | GLN  |
| 1   | J     | 944  | ASN  |
| 1   | J     | 988  | HIS  |
| 1   | J     | 1074 | GLN  |
| 1   | J     | 1100 | HIS  |
| 1   | J     | 1114 | GLN  |
| 1   | J     | 1159 | HIS  |
| 1   | J     | 1248 | HIS  |
| 1   | J     | 1267 | GLN  |
| 1   | J     | 1329 | GLN  |
| 1   | J     | 1366 | HIS  |
| 1   | J     | 1376 | HIS  |
| 1   | L     | 129  | HIS  |
| 1   | L     | 195  | GLN  |
| 1   | L     | 214  | ASN  |
| 1   | L     | 267  | GLN  |
| 1   | L     | 414  | ASN  |
| 1   | L     | 429  | ASN  |
| 1   | L     | 461  | ASN  |
| 1   | L     | 480  | HIS  |
| 1   | L     | 560  | ASN  |
| 1   | L     | 578  | GLN  |
| 1   | L     | 683  | ASN  |
| 1   | L     | 712  | GLN  |
| 1   | L     | 713  | HIS  |
| 1   | L     | 741  | ASN  |
| 1   | L     | 782  | GLN  |
| 1   | L     | 820  | HIS  |
| 1   | L     | 885  | HIS  |
| 1   | L     | 944  | ASN  |
| 1   | L     | 997  | ASN  |
| 1   | L     | 1017 | HIS  |
| 1   | L     | 1058 | GLN  |
| 1   | L     | 1081 | GLN  |
| 1   | L     | 1096 | GLN  |
| 1   | L     | 1098 | GLN  |
| 1   | L     | 1118 | HIS  |
| 1   | L     | 1159 | HIS  |
| 1   | L     | 1216 | GLN  |
| 1   | L     | 1366 | HIS  |
| 2   | M     | 15   | ASN  |
| 3   | N     | 124  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | N     | 137 | HIS  |
| 3   | N     | 147 | HIS  |
| 3   | N     | 282 | GLN  |
| 3   | N     | 461 | ASN  |
| 4   | O     | 38  | HIS  |
| 4   | O     | 207 | ASN  |
| 4   | O     | 232 | HIS  |
| 4   | P     | 85  | HIS  |
| 3   | Q     | 124 | GLN  |
| 3   | Q     | 137 | HIS  |
| 3   | Q     | 365 | ASN  |
| 3   | Q     | 479 | ASN  |
| 4   | R     | 24  | GLN  |
| 4   | R     | 38  | HIS  |
| 4   | R     | 108 | ASN  |
| 4   | R     | 193 | HIS  |
| 4   | R     | 229 | GLN  |
| 4   | R     | 315 | GLN  |
| 4   | S     | 108 | ASN  |
| 5   | T     | 18  | HIS  |
| 5   | T     | 83  | ASN  |
| 5   | T     | 95  | HIS  |
| 5   | T     | 101 | HIS  |
| 5   | T     | 197 | HIS  |
| 5   | T     | 234 | ASN  |
| 5   | T     | 235 | ASN  |
| 5   | T     | 250 | ASN  |
| 5   | T     | 376 | ASN  |
| 5   | T     | 410 | ASN  |
| 5   | T     | 412 | GLN  |
| 5   | T     | 434 | ASN  |
| 5   | T     | 451 | ASN  |
| 5   | T     | 628 | ASN  |
| 5   | T     | 632 | GLN  |
| 6   | U     | 144 | GLN  |
| 6   | U     | 207 | ASN  |
| 6   | U     | 302 | GLN  |
| 6   | U     | 328 | ASN  |
| 6   | U     | 332 | ASN  |
| 6   | U     | 401 | GLN  |
| 6   | U     | 451 | ASN  |
| 6   | U     | 473 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | U     | 528 | GLN  |
| 6   | U     | 539 | GLN  |
| 6   | V     | 244 | ASN  |
| 6   | V     | 359 | ASN  |
| 6   | V     | 433 | ASN  |
| 6   | V     | 435 | ASN  |
| 6   | V     | 492 | GLN  |
| 7   | W     | 35  | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

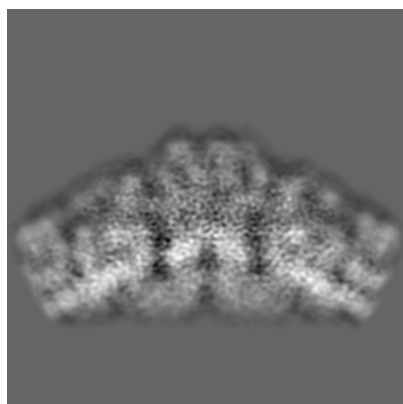
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49591. These allow visual inspection of the internal detail of the map and identification of artifacts.

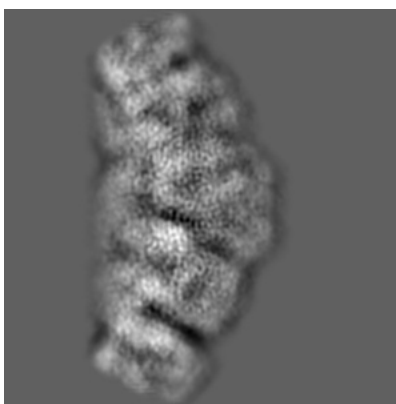
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

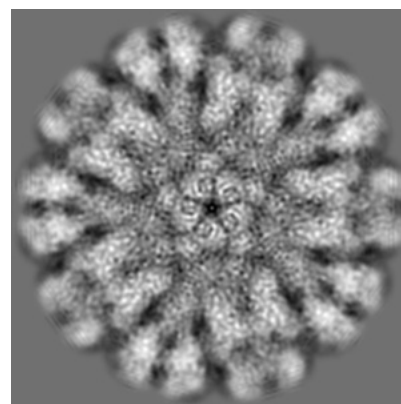
#### 6.1.1 Primary map



X

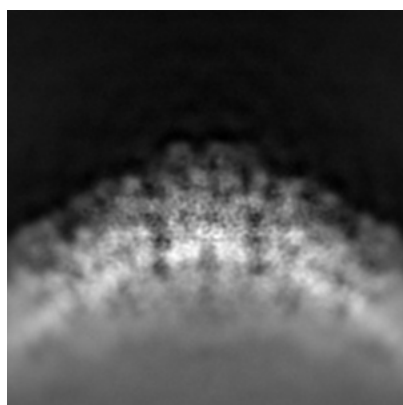


Y

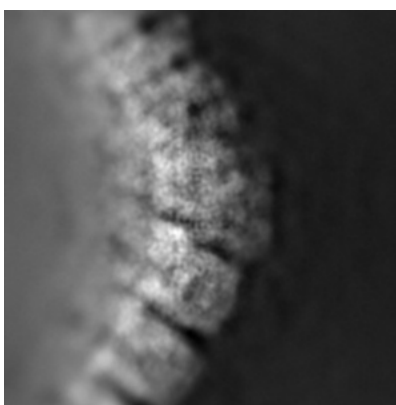


Z

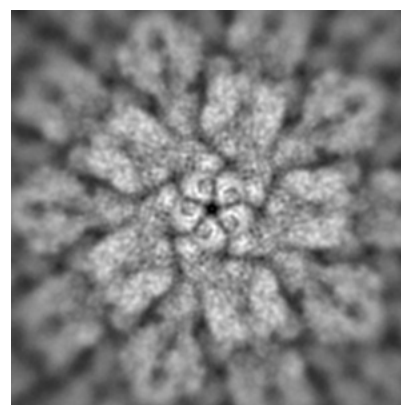
#### 6.1.2 Raw map



X



Y

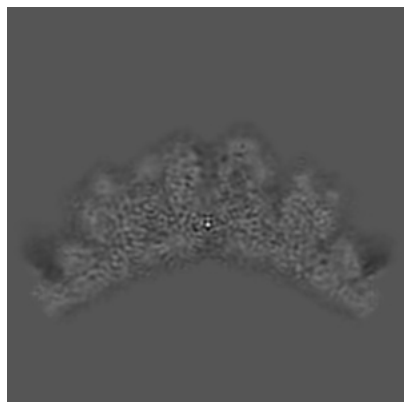


Z

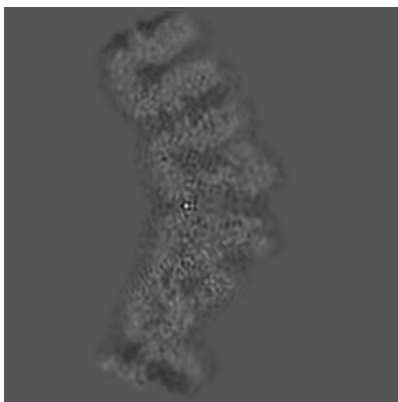
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

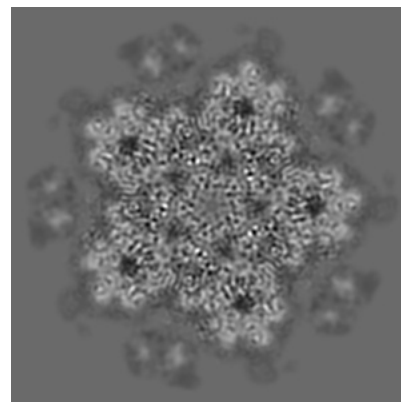
### 6.2.1 Primary map



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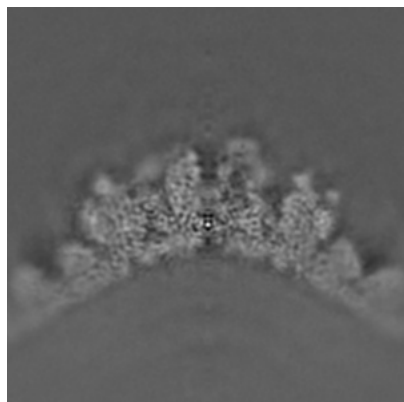


Y Index: 96

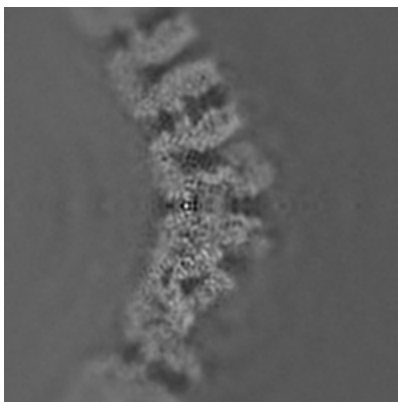


Z Index: 96

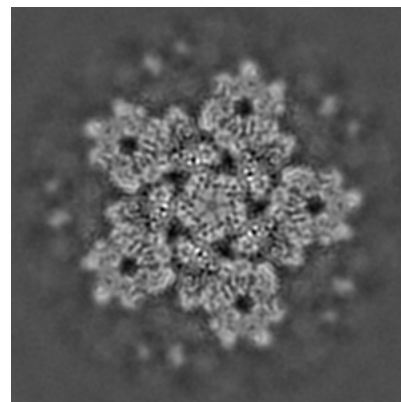
### 6.2.2 Raw map



X Index: 96



Y Index: 96

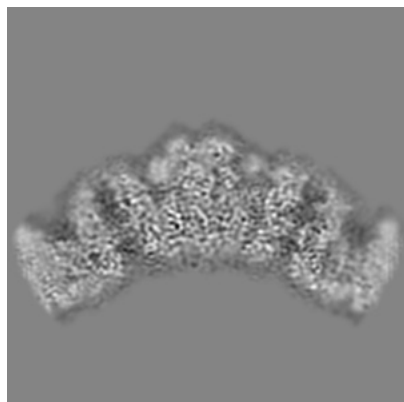


Z Index: 96

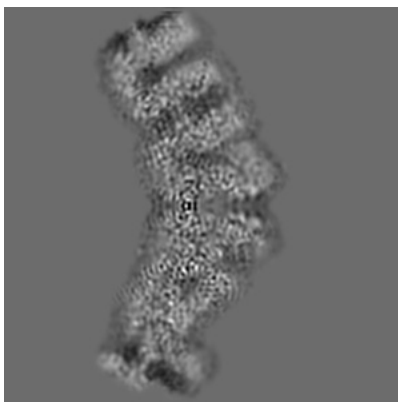
The images above show central slices of the map in three orthogonal directions.

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

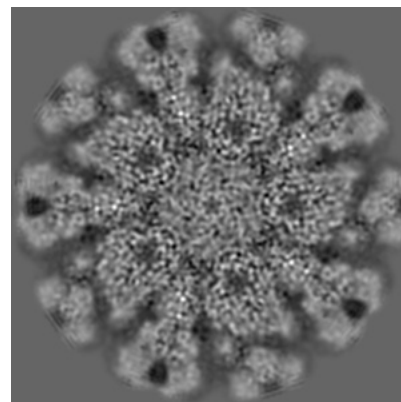
### 6.3.1 Primary map



X Index: 110

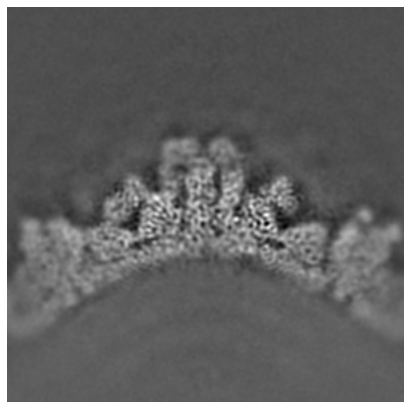


Y Index: 95

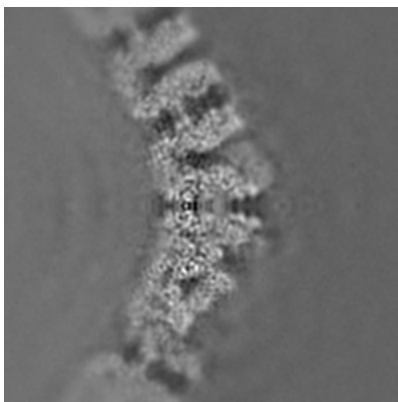


Z Index: 80

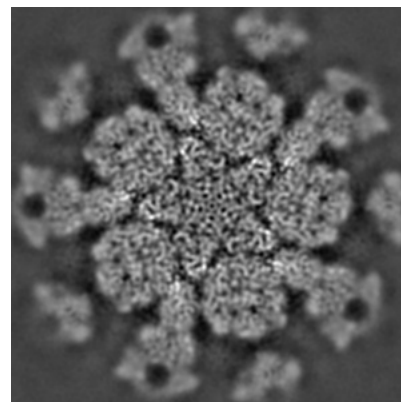
### 6.3.2 Raw map



X Index: 85



Y Index: 95

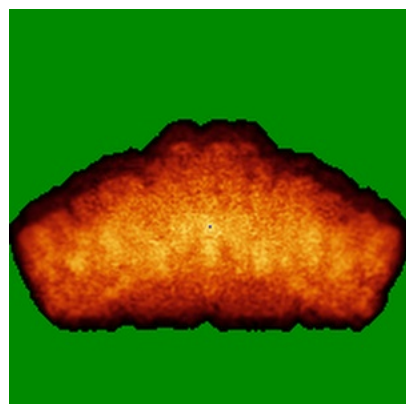


Z Index: 84

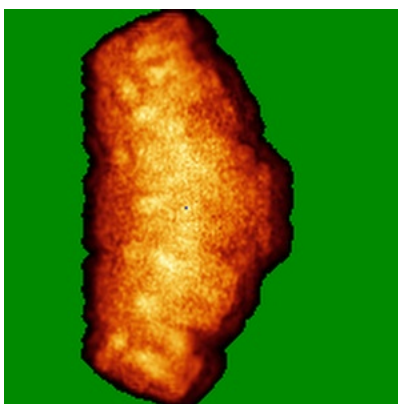
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X

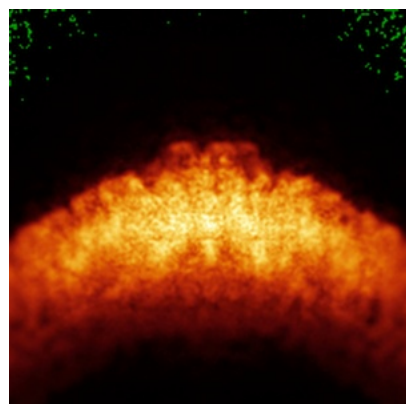


Y

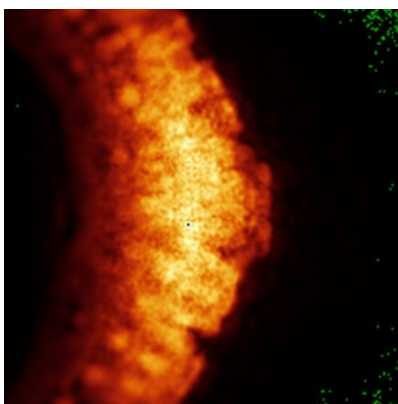


Z

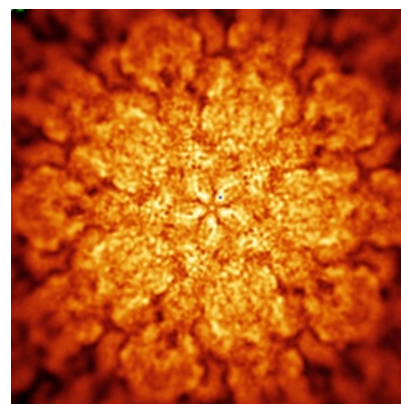
### 6.4.2 Raw map



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.

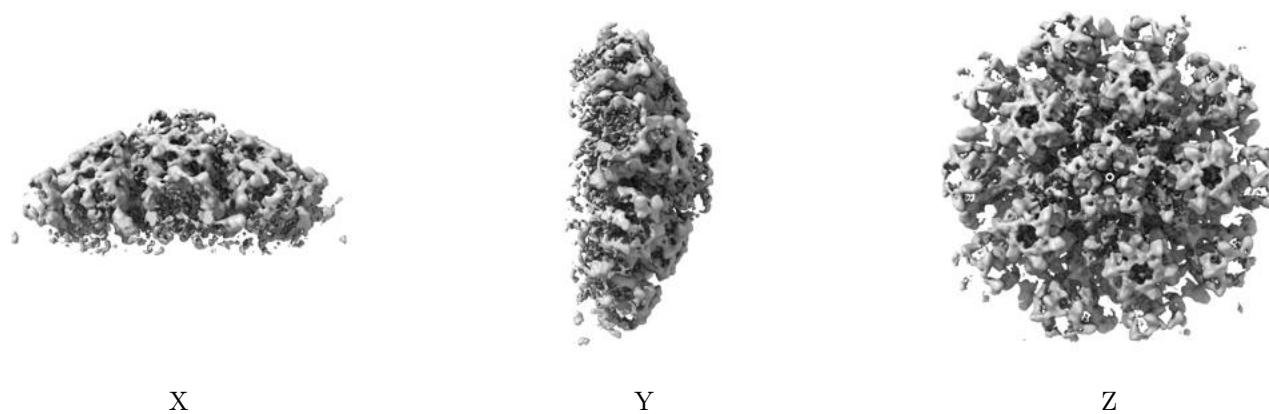
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.05. 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.

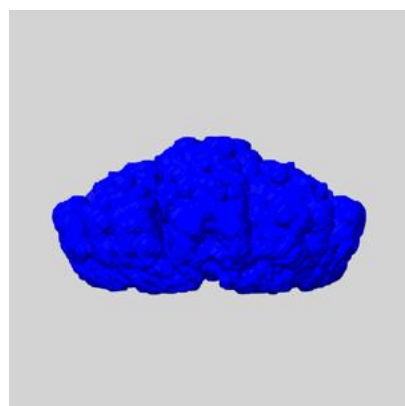
## 6.6 Mask visualisation [i](#)

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

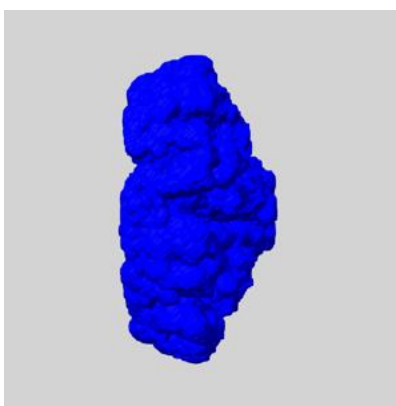
A mask typically either:

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

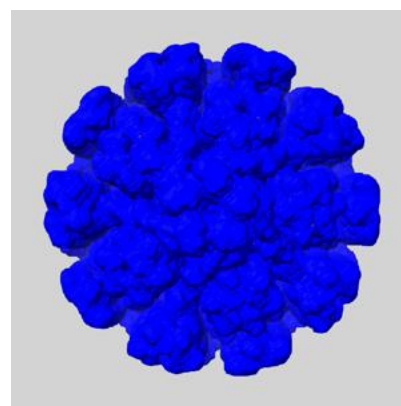
### 6.6.1 emd\_49591\_msk\_1.map [i](#)



X



Y

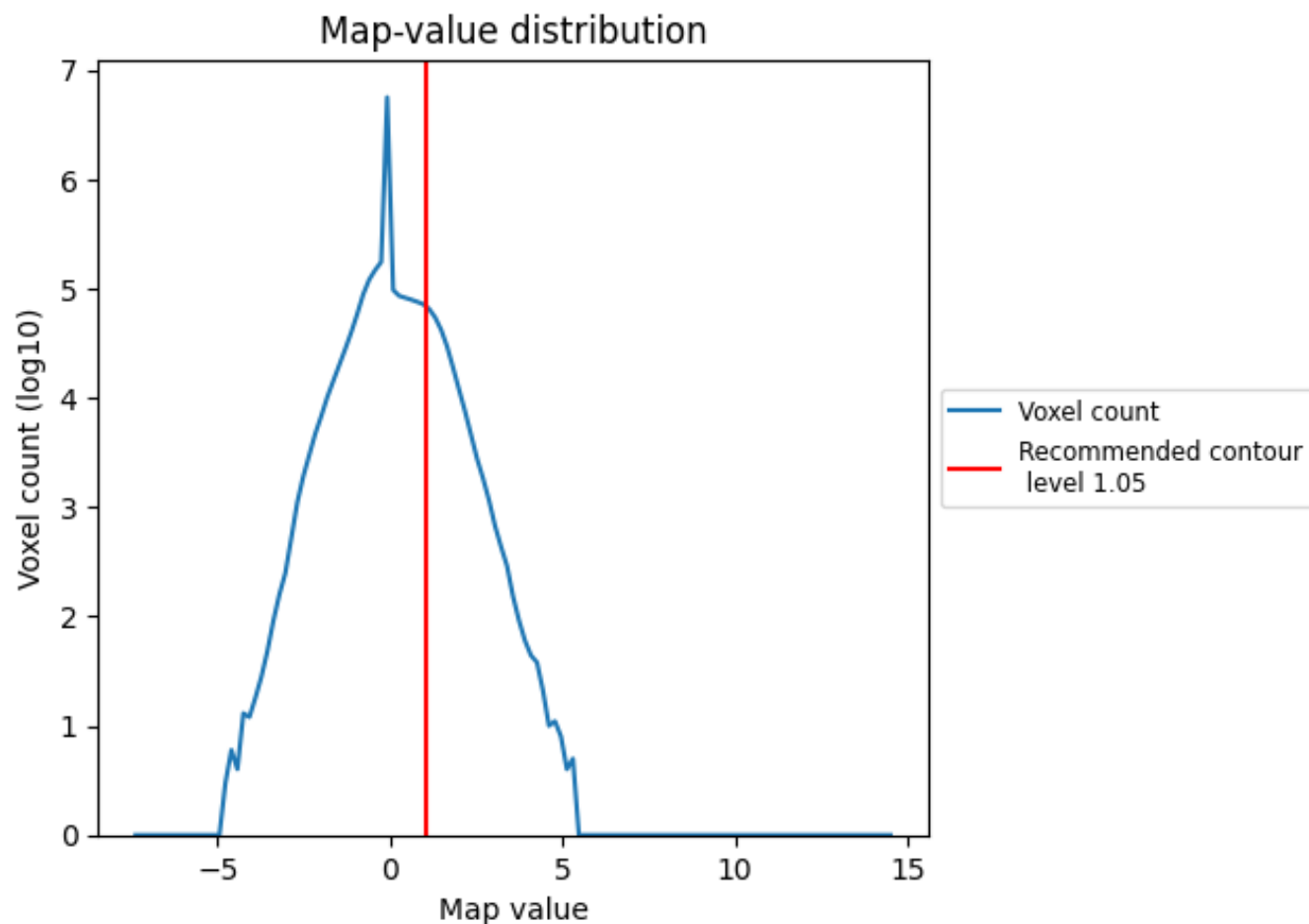


Z

## 7 Map analysis [i](#)

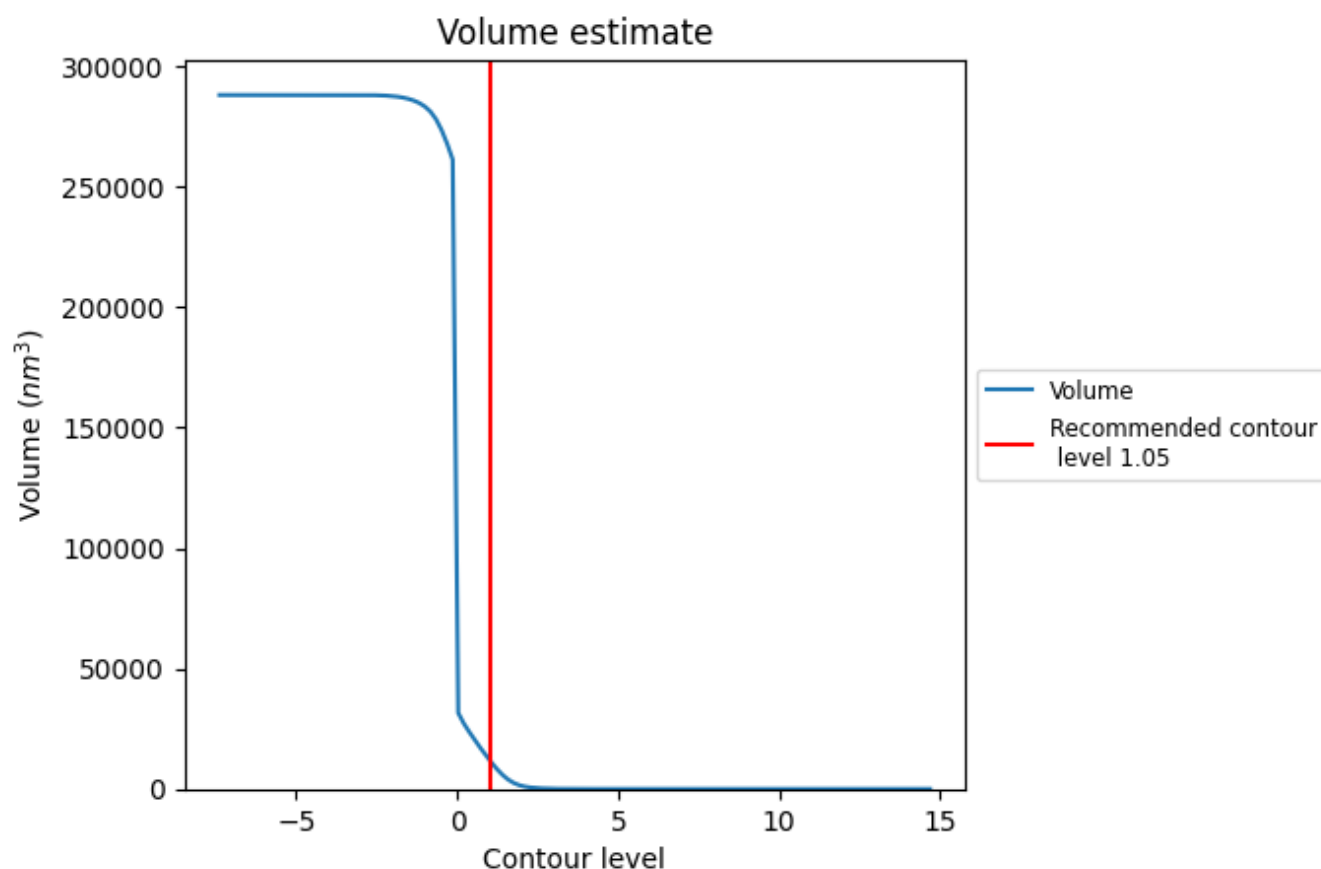
This section contains the results of statistical analysis of the map.

### 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.

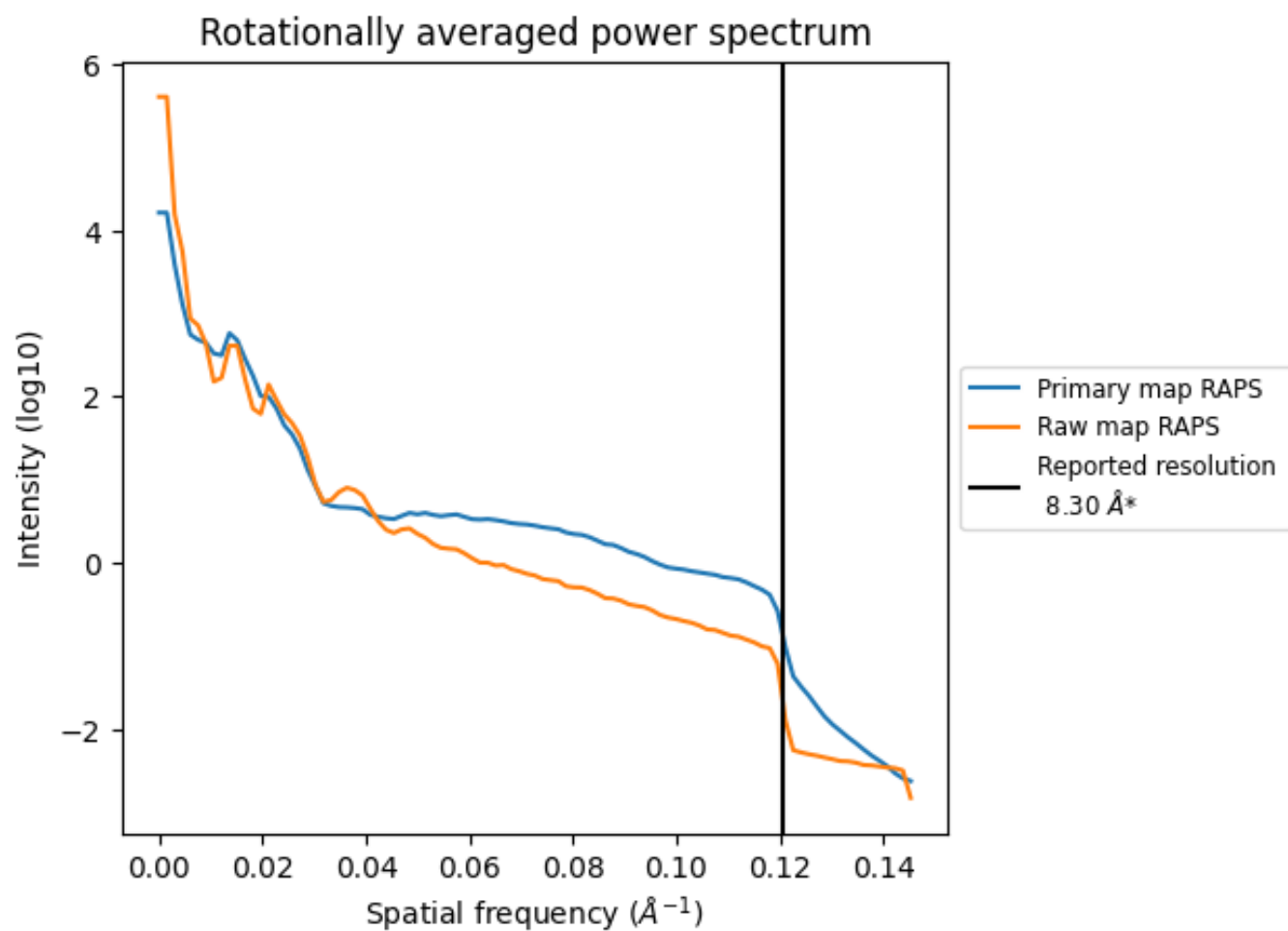
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11235  $\text{nm}^3$ ; this corresponds to an approximate mass of 10149 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 ⓘ

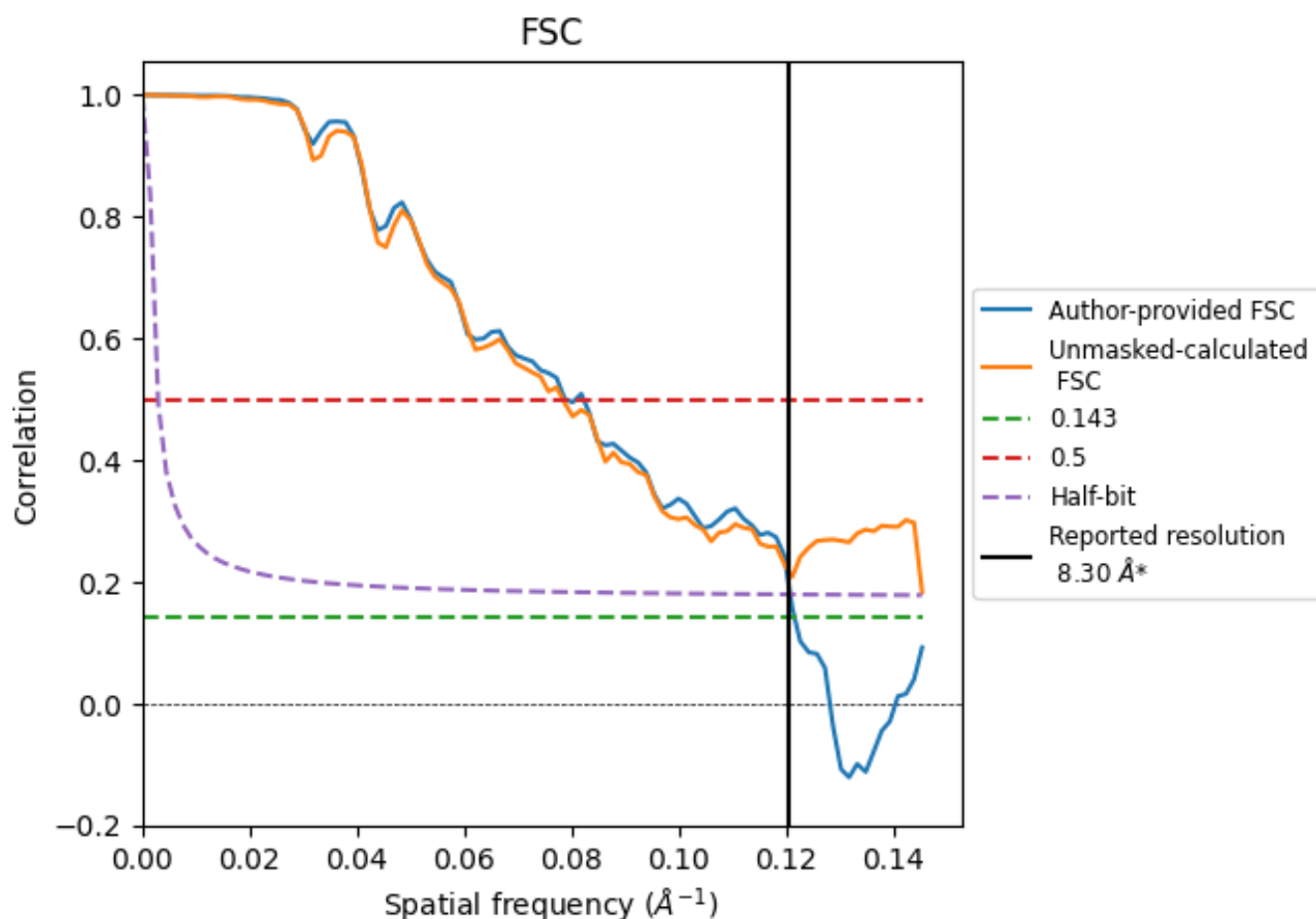


\*Reported resolution corresponds to spatial frequency of 0.120 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

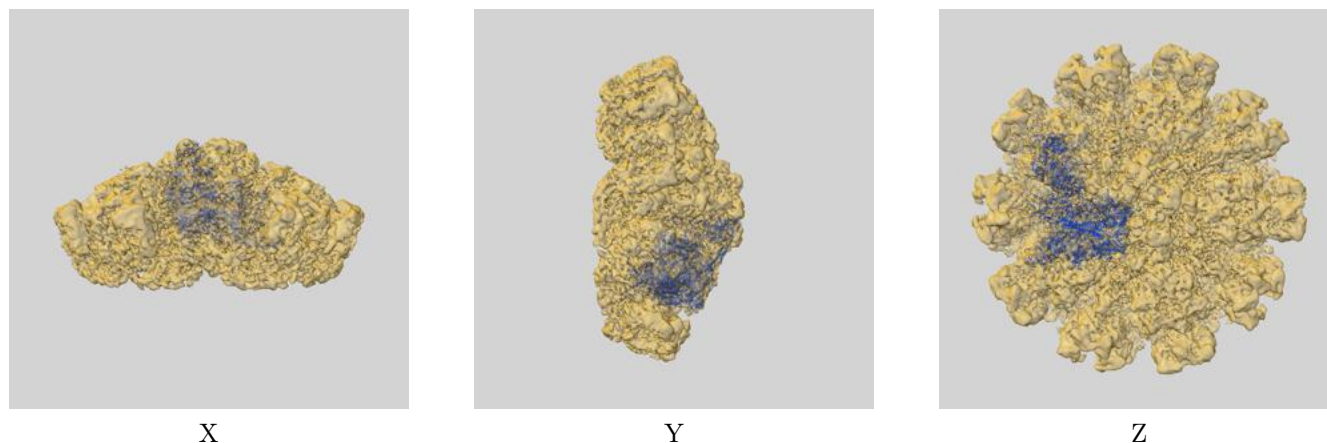
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 8.30                               | -     | -        |
| Author-provided FSC curve | 8.23                               | 12.67 | 8.29     |
| Unmasked-calculated*      | -                                  | 12.76 | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

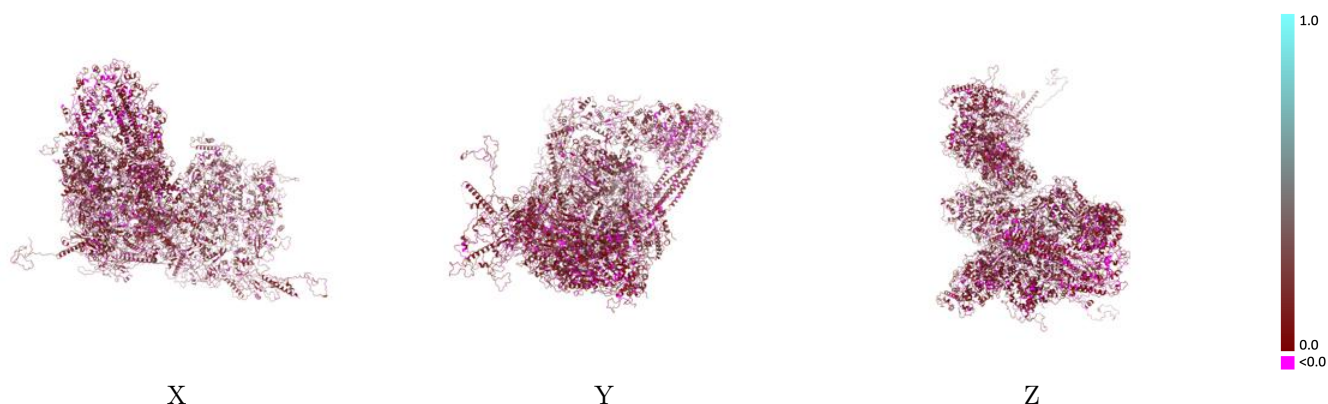
This section contains information regarding the fit between EMDB map EMD-49591 and PDB model 9NO1. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

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



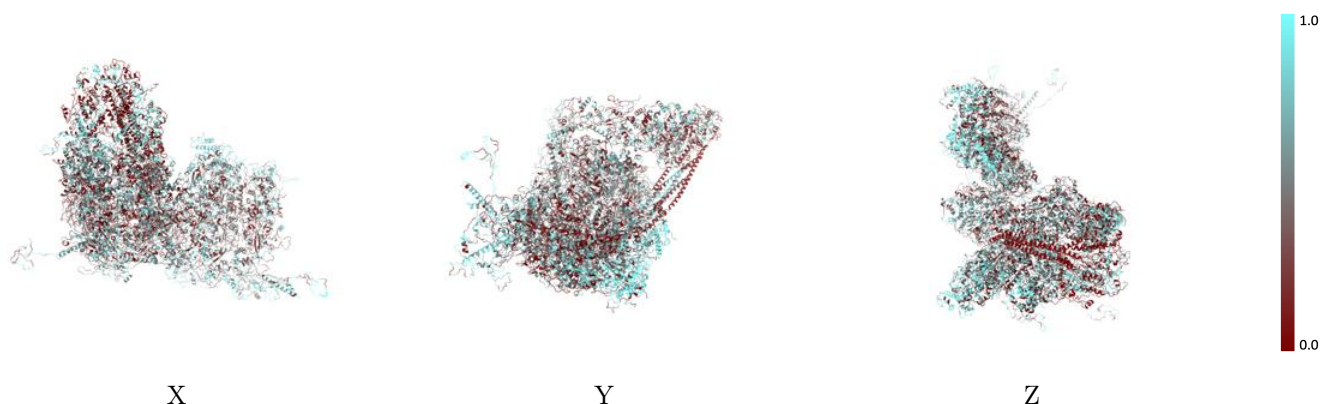
The images above show the 3D surface view of the map at the recommended contour level 1.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



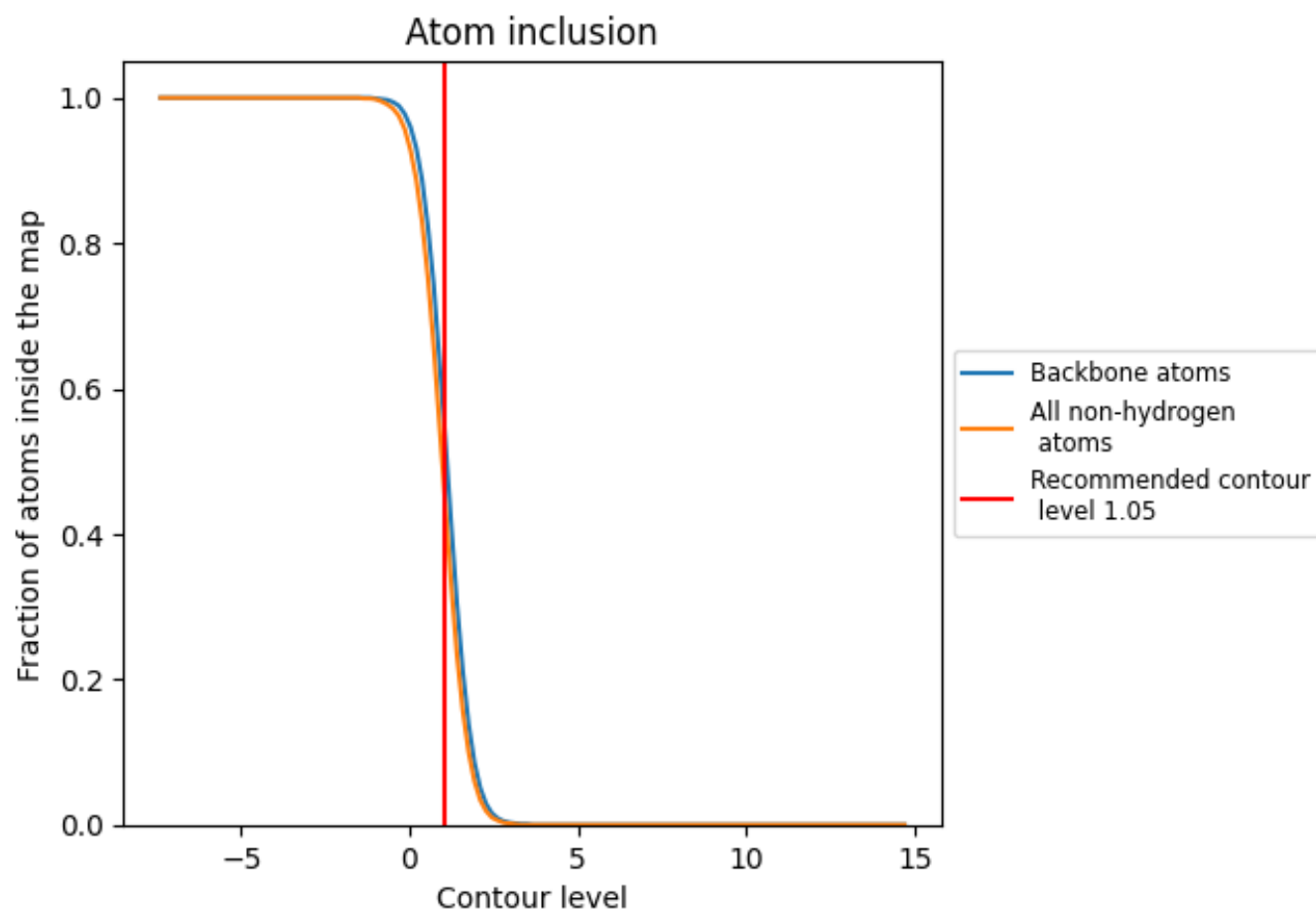
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.05).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 45% 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 (1.05) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.4500   |  0.1170   |
| A     |  0.4480   |  0.1270   |
| B     |  0.4660   |  0.1120   |
| C     |  0.6990   |  0.1060   |
| D     |  0.4970   |  0.1200   |
| E     |  0.7370   |  0.1210   |
| F     |  0.4660   |  0.1290   |
| G     |  0.7680   |  0.1510   |
| H     |  0.5030   |  0.1200   |
| I     |  0.7670   |  0.1270   |
| J     |  0.4240   |  0.1150   |
| K     |  0.6740   |  0.1120   |
| L     |  0.4480   |  0.1240   |
| M     |  0.7050   |  0.1240   |
| N     |  0.4170  |  0.1370  |
| O     |  0.4160 |  0.1400 |
| P     |  0.4080 |  0.1430 |
| Q     |  0.4900 |  0.1210 |
| R     |  0.4150 |  0.1290 |
| S     |  0.4190 |  0.1410 |
| T     |  0.3260 |  0.1100 |
| U     |  0.2520 |  0.0660 |
| V     |  0.3440 |  0.0490 |
| W     |  0.5400 |  0.1040 |
| X     |  0.0920 |  0.0440 |

